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# Simple Schemas for Unordered XML 

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#### Abstract

We consider unordered XML, where the relative order among siblings is ignored, and propose two simple yet practical schema formalisms: disjunctive multiplicity schemas (DMS), and its restriction, disjunction-free multiplicity schemas (MS). We investigate their computational properties and characterize the complexity of the following static analysis problems: schema satisfiability, membership of a tree to the language of a schema, schema containment, twig query satisfiability, implication, and containment in the presence of schema. Our research indicates that the proposed formalisms retain much of the expressiveness of DTDs without an increase in computational complexity.


## 1 Introduction

When XML is used for document-centric applications, the relative order among the elements is typically important e.g., the relative order of paragraphs and chapters in a book. On the other hand, in case of data-centric XML applications, the order among the elements may be unimportant [1. In this paper we focus on the latter use case. As an example, take a trivialized fragment of an XML document containing the DBLP repository in Figure 1 While the order of the elements title, author, and year may differ from one publication to another, it has no impact on the semantics of the data stored in this semi-structured database.

A schema for XML is a description of the type of admissible documents, typically defining for every node its content model i.e., the children nodes it must, may, or cannot contain. For instance, in the DBLP example, we shall require every article to have exactly one title, one year, and one or more author's. A book may additionally contain one publisher and may also have one or more editor's instead of author's. A schema has numerous important uses. For instance, it allows to validate a document against a schema and identify potential errors. A schema also serves as a reference for any user who does not know yet the structure of the XML document and attempts to query or modify its contents.

The Document Type Definition (DTD), the most widespread XML schema formalism for (ordered) XML [6, 13], is essentially a set of rules associating with each label a regular expression that defines the admissible sequences of children. The DTDs are best fitted towards ordered content because they use regular expressions, a formalism that defines sequences of labels. However, when unordered content model needs to be defined, there is a tendency to use over-permissive regular expressions. For instance, the DTD below corresponds to the one used in practice for the DBLP repository:

$$
\begin{aligned}
\text { dblp } & \rightarrow \text { (article } \mid \text { book) }^{*} \\
\text { article } & \rightarrow \text { (title } \mid \text { year } \mid \text { author)* } \\
\text { book } & \rightarrow \text { (title } \mid \text { year } \mid \text { author } \mid \text { editor } \mid \text { publisher) }{ }^{*}
\end{aligned}
$$



Figure 1: A trivialized DBLP repository.

This DTD allows an article to contain any number of title, year, and author elements. A book may also have any number of title, year, author, editor, and publisher elements. These regular expressions are clearly over-permissive because they allow documents that do not follow the intuitive guidelines set out earlier e.g., a document containing an article with two title's and no author should not be admissible.

While it is possible to capture unordered content models with regular expressions, a simple pumping argument shows that their size may need to be exponential in the number of possible labels of the children. In case of the DBLP repository, this number reaches values up to 12 , which basically precludes any practical use of such regular expressions. This suggests that overpermissive regular expressions may be employed for the reasons of conciseness and readability.

The use of over-permissive regular expressions, apart from allowing documents that do not follow the guidelines, has other negative consequences e.g., in static analysis tasks that involve the schema. Take for example the following two twig queries [2, 25]:

$$
\begin{aligned}
& \text { /dblp/book }[\text { author }=\text { "C. Papadimitriou"] } \\
& / \text { dblp/book }[\text { author }=\text { "C. Papadimitriou"][title }]
\end{aligned}
$$

The first query selects the elements labeled book, children of dblp and having an author containing the text "C. Papadimitriou." The second query additionally requires that book has a title. Naturally, these two queries should be equivalent because every book element should have a title child. However, the DTD above does not capture properly this requirement, and, consequently, the two queries are not equivalent w.r.t. this DTD.

In this paper, we study two new schema formalisms: the disjunctive multiplicity schema (DMS) and its restriction, the disjunction-free multiplicity schema (MS). While they use a userfriendly syntax inspired by DTDs, they define unordered content model only, and, therefore, they are better suited for unordered XML. A DMS is a set of rules associating with each label the possible number of occurrences for all the allowed children labels by using multiplicities: "*" (0 or more occurrences), "+" (1 or more), "?" (0 or 1 ), " 1 " (exactly 1 occurrence; often omitted for brevity). Additionally, alternatives can be specified using restricted disjunction ("|") and all the conditions are gathered with unordered concatenation ("\|"). For instance, the following DMS captures precisely the intuitive requirements for the DBLP repository:

$$
\begin{aligned}
\text { dblp } & \rightarrow \text { article* } \| \text { book* } \\
\text { article } & \rightarrow \text { title \|year \| author }{ }^{+} \\
\text {book } & \left.\rightarrow \text { title \|year \| publisher }{ }^{?} \| \text { (author }^{+} \mid \text {editor }^{+}\right)
\end{aligned}
$$

In particular, an article must have exactly one title, exactly one year, and at least one author. A book may additionally have a publisher and may have one or more editor's instead of author's.

| Problem of interest | DTD | DMS | disjunction-free DTD | MS |
| :---: | :---: | :---: | :---: | :---: |
| Schema satisfiability | PTIME [9, 21] | PTIME (Prop. 4.7) | PTIME [9, 21] | PTIME (Prop. 4.7) |
| Membership | PTIME [9, 21] | PTIME (Prop. 4.7) | PTIME 9, 21] | PTIME (Prop. 4.7) |
| Schema containment | PSPACE-c ${ }^{\dagger}$ /PTIME [9, 21] | PTIME (Th. 4.6) | coNP-h ${ }^{\dagger}$ /PTIME [9, 16] | PTIME (Th. 4.6) |
| Query satisfiability ${ }^{\ddagger}$ | NP-c [4] | NP-c (Prop. 4.8) | PTIME [4] | PTIME (Th. 4.16) |
| Query implication ${ }^{\ddagger}$ | EXPTIME-c [19] | EXPTIME-c (Prop. 4.9) | PTIME (Cor. 4.18) | PTIME (Th. 4.16) |
| Query containment ${ }^{\ddagger}$ | EXPTIME-c [19] | EXPTIME-c (Prop. 4.9) | coNP-c (Cor. 4.18) | coNP-c (Th. 4.17) |

${ }^{\dagger}$ when non-deterministic regular expressions are used. ${ }^{\ddagger}$ for twig queries.
Table 1: Summary of complexity results.

Note that, unlike the DTD defined earlier, this DMS does not allow documents having an article with several title's or without any author.

There has been an attempt to use DTD-like rule based schemas to define unordered content models by interpreting the regular expressions under commutative closure [3: essentially, an unordered collection of children matches a regular expression if there exists an ordering that matches the regular expression in the standard way. However, testing whether there exists a permutation of a word that matches a regular expression is NP-complete [15], which implies a significant increase in computational complexity of the membership problem i.e., validating an XML document against the schema. The schema formalisms proposed in this paper, DMS and MS, can be seen as DTDs interpreted under commutative closure using restricted classes of regular expressions. Two natural questions arise: do these restrictions allow us to avoid the increase in computational complexity, and how much of the expressiveness of DTDs is retained. The answers are generally positive. There is no increase in computational complexity but also no decrease (cf. Table 1). Furthermore, the proposed schema formalisms seem to capture a significant part of the expressiveness of DTDs used in practice (Section 5).

We study the complexity of several basic decision problems: schema satisfiability, membership of a tree to the language of a schema, containment of two schemas, twig query satisfiability, implication, and containment in the presence of schema. Table 1 contains the summary of complexity results compared with general DTDs and disjunction-free DTDs. The lower bounds for the decision problems for DMS and MS are generally obtained with easy adaptations of their counterparts for general DTDs and disjunction-free DTDs. To obtain upper bounds we develop several new tools. Dependency graphs for MS and a generalized definition of an embedding of a query help us to reason about query satisfiability, query implication, and query containment in the presence of MS. An alternative characterization of DMS with characterizing triples is used to reduce the containment of DMS to the containment of their characterizing triples, which can be tested in PTIME. We add that our constructions and results for MS extend easily to disjunctionfree DTDs and allow to solve the problems of query implication and query containment, which, to the best of our knowledge, have not been previously studied for disjunction-free DTDs.
Related work. Languages of unordered trees can be expressed by logic formalisms or by tree automata. Boneva et al. [7, 8] make a survey on such formalisms and compare their expressiveness. The fundamental difference resides in the kind of constraints that can be expressed for the allowed collections of children for some node. We mention here only formalisms introduced in the context of XML. Presburger automata [24, sheaves automata [11, and the TQL logic [10] allow to express Presburger constraints on the numbers of occurrences of the different symbols among the children of some node. This is also equivalent to considering DTDs under commutative closure, similarly to 3. The consequence of the high expressive power is that the membership problem is NPcomplete for an unbounded alphabet 15. Therefore, these formalisms were not extensively used in practice. Suitable restrictions on Presburger automata and on the TQL logic allow to
obtain the same expressiveness as the MSO logic on unordered trees [7, 8. DMS are strictly less expressive than these MSO-equivalent languages. Static analysis problems involving twig queries were not studied for these languages. Additionally, we believe that DMS are more appropriate to be used as schema languages, as they were designed as such, in particular regarding the more user-friendly DTD-like syntax. As mentioned earlier, unordered content model can also be defined by DTDs defining commutatively-closed sets of ordered trees. An (ordered) tree matches such a DTD iff all tree obtained by reordering of sibling nodes also matches the DTD. This also turns out to be equally expressive as MSO on unordered trees [7, 8. However, such a DTD may be of exponential size w.r.t. the size of the alphabet and, moreover, it is PSPACE-complete to test whether a DTD defines a commutatively-closed set of trees [18], which makes such DTDs unusable in practice. XML Schema allow for a bounded number of symbols to appear in arbitrary order, and RELAX NG allows to interleave sequences of symbols of bounded length. In contrast, the Kleene star in DMS allows for unbounded unordered collections of children. Schematron allows to specify very general constraints on the number of occurrences of symbols among the children of a node, in particular Presburger constraints are expressible. Schema languages using regular expressions with unbounded interleaving were studied in [12]. These are more expressive than DMS but exhibit high computational complexity of inclusion [12] and membership [5]. To the best of our knowledge, the static analysis problems involving queries were not studied for these languages when unordered content is allowed.
Organization. The paper is organized as follows. In Section 2 we introduce some preliminary notions, while in Section 3we present our schema formalisms. In Section 4 we define the problems of interest and then we analyze them for DMS (Subsection 4.1) and for MS (Subsection 4.2). In Section 5 we discuss the expressiveness of the proposed formalisms, while in Section 6 we summarize our results and outline further directions. Because of space restriction, we present only sketches of some proofs; complete proofs will be given in the full version of the paper, which is currently in preparation for journal submission.

## 2 Preliminaries

Throughout this paper we assume an alphabet $\Sigma$ which is a finite set of symbols.
Trees. We model XML documents with unordered labeled trees. Formally, a tree $t$ is a tuple $\left(N_{t}\right.$, root $_{t}$, lab $_{t}$, child $\left._{t}\right)$, where $N_{t}$ is a finite set of nodes, root $_{t} \in N_{t}$ is a distinguished root node, $l a b_{t}: N_{t} \rightarrow \Sigma$ is a labeling function, and child ${ }_{t} \subseteq N_{t} \times N_{t}$ is the parent-child relation. We assume that the relation child $_{t}$ is acyclic and require every non-root node to have exactly one predecessor in this relation. By Tree we denote the set of all finite trees.

(a) Tree $t_{0}$.

(b) Twig query $q_{0}$.

Figure 2: A tree and a twig query.
Queries. We work with the class of twig queries, which are essentially unordered trees whose nodes may be additionally labeled with a distinguished wildcard symbol $\star \notin \Sigma$ and that use two
types of edges, child (/) and descendant (//), corresponding to the standard XPath axes. Note that the semantics of $/ /$-edge is that of a proper descendant (and not that of descendant-or-self). Formally, a twig query $q$ is a tuple ( $\left.N_{q}, \operatorname{root}_{q}, \operatorname{lab}_{q}, \operatorname{child}_{q}, \operatorname{desc}_{q}\right)$, where $N_{q}$ is a finite set of nodes, $\operatorname{root}_{q} \in N_{q}$ is the root node, $\operatorname{lab}_{q}: N_{q} \rightarrow \Sigma \cup\{\star\}$ is a labeling function, child ${ }_{q} \subseteq N_{q} \times N_{q}$ is a set of child edges, and $\operatorname{desc}_{q} \subseteq N_{q} \times N_{q}$ is a set of descendant edges. We assume that child $_{q} \cap \operatorname{desc}_{q}=\varnothing$ and that the relation $\operatorname{child}_{q} \cup \operatorname{desc}_{q}$ is acyclic and we require every non-root node to have exactly one predecessor in this relation. By Twig we denote the set of all twig queries. Twig queries are often presented using the abbreviated XPath syntax 25 e.g., the query $q_{0}$ in Figure 2(b) can be written as $r / \star[\star] / / a$.
Embeddings. We define the semantics of twig queries using the notion of embedding which is essentially a mapping of nodes of a query to the nodes of a tree that respects the semantics of the edges of the query. Formally, for a query $q \in$ Twig and a tree $t \in$ Tree, an embedding of $q$ in $t$ is a function $\lambda: N_{q} \rightarrow N_{t}$ such that:

1. $\lambda\left(\operatorname{root}_{q}\right)=$ root $_{t}$,
2. for every $\left(n, n^{\prime}\right) \in \operatorname{child}_{q},\left(\lambda(n), \lambda\left(n^{\prime}\right)\right) \in \operatorname{child}_{t}$,
3. for every $\left(n, n^{\prime}\right) \in \operatorname{desc}_{q},\left(\lambda(n), \lambda\left(n^{\prime}\right)\right) \in\left(\text { child }_{t}\right)^{+}$(the transitive closure of child $\left.{ }_{t}\right)$,
4. for every $n \in N_{q}, l a b_{q}(n)=\star$ or $l a b_{q}(n)=l a b_{t}(\lambda(n))$.

If there exists an embedding from $q$ to $t$ we say that $t$ satisfies $q$ and we write $t \models q$. By $L(q)$ we denote the set of all the trees satisfying $q$. Note that we do not require the embedding to be injective i.e., two nodes of the query may be mapped to the same node of the tree. Figure 3 presents all embeddings of the query $q_{0}$ in the tree $t_{0}$ from Figure 2


Figure 3: Embeddings of $q_{0}$ in $t_{0}$.
Unordered words. An unordered word is essentially a multiset of symbols i.e., a function $w: \Sigma \rightarrow \mathbb{N}_{0}$ mapping symbols from the alphabet to natural numbers, and we call the number $w(a)$ the number of occurrences of the symbol $a$ in $w$. We also write $a \in w$ as a shorthand for $w(a) \neq 0$. An empty word $\varepsilon$ is an unordered word that has 0 occurrences of every symbol i.e., $\varepsilon(a)=0$ for every $a \in \Sigma$. We often use a simple representation of unordered words, writing each symbol in the alphabet the number of times it occurs in the unordered word. For example, when the alphabet is $\Sigma=\{a, b, c\}, w_{0}=a a a c c$ stands for the function $w_{0}(a)=3, w_{0}(b)=0$, and $w_{0}(c)=2$.

The (unordered) concatenation of two unordered words $w_{1}$ and $w_{2}$ is defined as the multiset union $w_{1} \uplus w_{2}$ i.e., the function defined as $\left(w_{1} \uplus w_{2}\right)(a)=w_{1}(a)+w_{2}(a)$ for all $a \in \Sigma$. For instance, $a a a c c \uplus a b b c=a a a a b b c c c$. Note that $\varepsilon$ is the identity element of the unordered concatenation $\varepsilon \uplus w=w \uplus \varepsilon=w$ for all unordered word $w$. Also, given an unordered word $w$, by $w^{i}$ we denote the concatenation $w \uplus \ldots \uplus w(i$ times $)$.

A language is a set of unordered words. The unordered concatenation of two languages $L_{1}$ and $L_{2}$ is a language $L_{1} \uplus L_{2}=\left\{w_{1} \uplus w_{2} \mid w_{1} \in L_{1}, w_{2} \in L_{2}\right\}$. For instance, if $L_{1}=\{a, a a c\}$ and $L_{2}=\{a c, b, \varepsilon\}$, then $L_{1} \uplus L_{2}=\{a, a b, a a c, a a b c, a a a c c\}$.

## 3 Multiplicity schemas

A multiplicity is an element from the set $\{*,+, ?, 0,1\}$. We define the function $\llbracket \rrbracket$ mapping multiplicities to sets of natural numbers. More precisely:

$$
\llbracket * \rrbracket=\{0,1,2, \ldots\}, \quad \llbracket+\rrbracket=\{1,2, \ldots\}, \quad \llbracket ? \rrbracket=\{0,1\}, \quad \llbracket 1 \rrbracket=\{1\}, \quad \llbracket 0 \rrbracket=\{0\} .
$$

Given a symbol $a \in \Sigma$ and a multiplicity $M$, the language of $a^{M}$, denoted $L\left(a^{M}\right)$, is $\left\{a^{i} \mid i \in \llbracket M \rrbracket\right\}$. For example, $L\left(a^{+}\right)=\{a, a a, \ldots\}, L\left(b^{0}\right)=\{\varepsilon\}$, and $L\left(c^{?}\right)=\{\varepsilon, c\}$.

A disjunctive multiplicity expression $E$ is:

$$
E:=D_{1}^{M_{1}}\|\ldots\| D_{n}^{M_{n}},
$$

where for all $1 \leqslant i \leqslant n, M_{i}$ is a multiplicity and each $D_{i}$ is:

$$
D_{i}:=a_{1}^{M_{1}^{\prime}}|\ldots| a_{k}^{M_{k}^{\prime}}
$$

where for all $1 \leqslant j \leqslant k, M_{j}^{\prime}$ is a multiplicity and $a_{j} \in \Sigma$. Moreover, we require that every symbol $a \in \Sigma$ is present at most once in a disjunctive multiplicity expression. For instance, $(a \mid b) \|(c \mid d)$ is a disjunctive multiplicity expression, but $(a \mid b)\|c\|(a \mid d)$ is not because $a$ appears twice. A disjunction-free multiplicity expression is an expression which uses no disjunction symbol "|" i.e., an expression of the form $a_{1}^{M_{1}}\|\ldots\| a_{k}^{M_{k}}$, where for all $1 \leqslant i \leqslant k$, the $a_{i}$ 's are pairwise distinct symbols in the alphabet and the $M_{i}$ 's are multiplicities.

The language of a disjunctive multiplicity expression is:

$$
\begin{gathered}
L\left(a_{1}^{M_{1}}|\ldots| a_{k}^{M_{k}}\right)=L\left(a_{1}^{M_{1}}\right) \cup \ldots \cup L\left(a_{k}^{M_{k}}\right), \\
L\left(D^{M}\right)=\left\{w_{1} \uplus \ldots \uplus w_{i} \mid w_{1}, \ldots, w_{i} \in L(D) \wedge i \in \llbracket M \rrbracket\right\}, \\
L\left(D_{1}^{M_{1}}\|\ldots\| D_{n}^{M_{n}}\right)=L\left(D_{1}^{M_{1}}\right) \uplus \ldots \uplus L\left(D_{n}^{M_{n}}\right) .
\end{gathered}
$$

If an unordered word $w$ belongs to the language of a disjunctive multiplicity expression $E$, we denote it $w \models E$. When a symbol $a$ (resp. a disjunctive multiplicity expression $E$ ) has multiplicity 1, we often write $a$ (resp. E) instead of $a^{1}$ (resp. $E^{1}$ ). Moreover, we omit writing symbols and disjunctive multiplicity expressions with multiplicity 0 . Take for instance, $E_{0}=a^{+}\|(b \mid c)\| d^{?}$ and note that both the symbols $b$ and $c$ as well as the disjunction $(b \mid c)$ have an implicit multiplicity 1. The language of $E_{0}$ is:

$$
L\left(E_{0}\right)=\left\{a^{i} b^{j} c^{k} d^{\ell} \mid i, j, k, \ell \in \mathbb{N}_{0}, i \geqslant 1, j+k=1, \ell \leqslant 1\right\}
$$

Next, we formally define the proposed schema formalisms.
Definition 3.1 $A$ disjunctive multiplicity schema (DMS) is a tuple $S=\left(\operatorname{root}_{S}, R_{S}\right)$, where root $_{S} \in \Sigma$ is a designated root label and $R_{S}$ maps symbols in $\Sigma$ to disjunctive multiplicity expressions. By DMS we denote the set of all disjunctive multiplicity schemas. A disjunction-free multiplicity schema (MS) $S=\left(\operatorname{root}_{S}, R_{S}\right)$ is a restriction of the DMS, where $R_{S}$ maps symbols in $\Sigma$ to disjunction-free multiplicity expressions. By MS we denote the set of all disjunction-free multiplicity schemas.
To define satisfiabily of a DMS (or MS) $S$ by a tree $t$ we first define the unordered word $c h_{t}^{n}$ of children of a node $n \in N_{t}$ of $t$ i.e., $c h_{t}^{n}(a)=\left|\left\{m \in N_{t} \mid(n, m) \in \operatorname{child}_{t} \wedge l a b_{t}(m)=a\right\}\right|$. Now, a tree $t$ satisfies $S$, in symbols $t \models S$, if $l a b_{t}\left(\operatorname{root}_{t}\right)=\operatorname{root}_{S}$ and for any node $n \in N_{t}$, $c h_{t}^{n} \in L\left(R_{S}\left(l a b_{t}(n)\right)\right)$. By $L(S) \subseteq$ Tree we denote the set of all the trees satisfying $S$.

In the sequel, we represent a schema $S=\left(\operatorname{root}_{S}, R_{S}\right)$ as a set of rules of the form $a \rightarrow R_{S}(a)$, for any $a \in \Sigma$. If $L\left(R_{S}(a)\right)=\varepsilon$, then we write $a \rightarrow \epsilon$ or we simply omit writing such a rule.

Example 3.2 We present schemas $S_{1}, S_{2}, S_{3}, S_{4}$ illustrating the formalisms defined above. They have the root label $r$ and the rules:

| $S_{1}:$ | $r \rightarrow a\left\\|b^{*}\right\\| c^{?}$ | $a \rightarrow b^{?}$ | $b \rightarrow a^{?}$ |
| :--- | :--- | :--- | :--- |
| $S_{2}:$ | $r \rightarrow c\\|b\\| a$ | $a \rightarrow b^{?}$ | $b \rightarrow a$ |
| $S_{3}:$ | $r \rightarrow(a \mid b)^{+} \\| c$ | $a \rightarrow b^{?}$ | $b \rightarrow a$ |
| $S_{4}:$ | $r \rightarrow(a\|b\| c)^{*}$ | $a \rightarrow \epsilon$ | $c \rightarrow b$ |

$S_{1}$ and $S_{2}$ are $M S$, while $S_{3}$ and $S_{4}$ are $D M S$. The tree $t_{0}$ from Figure 2(a) satisfies only $S_{1}$ and $S_{3}$.

## 4 Static analysis

We first define the problems of interest and we formally state the corresponding decision problems parameterized by the class of schema and, when appropriate, by a class of queries.
Schema satisfiability - checking if there exists a tree satisfying the given schema:

$$
\operatorname{SAT}_{\mathcal{S}}=\{S \in \mathcal{S} \mid \exists t \in \text { Tree. } t \models S\} .
$$

Membership - checking if the given tree satisfies the given schema:

$$
\operatorname{MEMB}_{\mathcal{S}}=\{(S, t) \in \mathcal{S} \times \text { Tree } \mid t \models S\}
$$

Schema containment - checking if every tree satisfying one given schema satisfies another given schema:

$$
\operatorname{CNT}_{\mathcal{S}}=\left\{\left(S_{1}, S_{2}\right) \in \mathcal{S} \times \mathcal{S} \mid L\left(S_{1}\right) \subseteq L\left(S_{2}\right)\right\}
$$

Query satisfiability by schema - checking if there exists a tree that satisfies the given schema and the given query:

$$
\operatorname{SAT}_{\mathcal{S}, \mathcal{Q}}=\{(S, q) \in \mathcal{S} \times \mathcal{Q} \mid \exists t \in L(S) . t \models q\}
$$

Query implication by schema - checking if every tree satisfying the given schema satisfies also the given query:

$$
\operatorname{IMPL}_{\mathcal{S}, \mathcal{Q}}=\{(S, q) \in \mathcal{S} \times \mathcal{Q} \mid \forall t \in L(S) . t \models q\}
$$

Query containment in the presence of schema - checking if every tree satisfying the given schema and one given query also satisfies another given query:

$$
\operatorname{CNT}_{\mathcal{S}, \mathcal{Q}}=\{(p, q, S) \in \mathcal{Q} \times \mathcal{Q} \times \mathcal{S} \mid \forall t \in L(S) . t \models p \Rightarrow t \models q\}
$$

We next study these decision problems for DMS an MS.

### 4.1 Disjunctive multiplicity schema

In this subsection we present the static analysis for DMS. We first introduce the notion of normalized disjunctive multiplicity expressions and an alternative definition with characterizing triples. Finally, we state the complexity results for DMS.

### 4.1.1 Normalized disjunctive multiplicity expressions

Recall that a disjunctive multiplicity expression has the form $E=D_{1}^{M_{1}}\|\ldots\| D_{m}^{M_{m}}$. Intuitively, in a normalized disjunctive multiplicity expression, every disjunction $D_{i}^{M_{i}}$ has one of the following three forms:

1. $\left(a_{1}|\ldots| a_{n}\right)^{+}$,
2. $\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right)$, where $\forall j .1 \leqslant j \leqslant n .0 \notin \llbracket M_{j} \rrbracket$,
3. $\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right)$, where $\forall j .1 \leqslant j \leqslant n .0 \in \llbracket M_{j} \rrbracket$.

Given a disjunctive multiplicity expression $E=D_{1}^{M_{1}}\|\ldots\| D_{m}^{M_{m}}$, we denote by $\Sigma_{D_{i}}$ the set of symbols used in the disjunction from $D_{i}$ and by $M^{a}$ the multiplicity corresponding to a symbol $a$. Formally, we say that $E$ is normalized if the following two conditions are satisfied:

$$
\begin{aligned}
& \forall i .1 \leqslant i \leqslant m . M_{i} \neq 1 \Rightarrow M_{i}=+\wedge \forall a \in \Sigma_{D_{i}} . M^{a}=1 \\
& \forall i .1 \leqslant i \leqslant m .\left(\exists a \in \Sigma_{D_{i}} .0 \in \llbracket M^{a} \rrbracket\right) \Rightarrow\left(\forall a^{\prime} \in \Sigma_{D_{i}} .0 \in \llbracket M^{a^{\prime}} \rrbracket\right)
\end{aligned}
$$

Any $D_{i}^{M_{i}}$ can be rewritten as an equivalent normalized disjunctive multiplicity expression using the following rules:

- $\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right)^{*}$ goes to $a_{1}^{*}\|\ldots\| a_{n}^{*}$.
- $\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right)^{\text {? }}$ goes to $\left(a_{1}^{M_{1}^{\prime}}|\ldots| a_{n}^{M_{n}^{\prime}}\right)$, where $\forall j .1 \leqslant j \leqslant n$. $\llbracket M_{j}^{\prime} \rrbracket=\{0\} \cup \llbracket M_{j} \rrbracket$.
- $\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right)$, where $\exists j .1 \leqslant j \leqslant n$. $0 \in \llbracket M_{j} \rrbracket$ goes to ( $a_{1}^{M_{1}^{\prime}}|\ldots| a_{n}^{M_{n}^{\prime}}$ ), where $\forall j .1 \leqslant j \leqslant n . \llbracket M_{j}^{\prime} \rrbracket=\{0\} \cup \llbracket M_{j} \rrbracket$.
- $\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right)^{+}$, where $\exists j .1 \leqslant j \leqslant n .0 \in \llbracket M_{j} \rrbracket$ goes to $a_{1}^{*}\|\ldots\| a_{n}^{*}$.
- $\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right)^{+}$, where $\forall j .1 \leqslant j \leqslant n .0 \notin \llbracket M_{j} \rrbracket$ goes to $\left(a_{1}|\ldots| a_{n}\right)^{+}$.
- $\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right)^{0}$ is removed.
- $a^{0}$ occurring in some disjunction is removed.

Note that each of the rewriting steps gives an equivalent expression. From now on, we assume w.l.o.g. that all the disjunctive multiplicity expressions that we manipulate are normalized.

### 4.1.2 Alternative definition with characterizing triples

We propose an alternative definition of the language of a disjunctive multiplicity expression using a characterizing triple. Moreover, we show that each element of the triple has a compact representation which is polynomial in the size of the alphabet and computable in PTIME. Recall that the disjunctive multiplicity expressions do not allow repetitions of symbols hence they have size linear in $|\Sigma|$. Next, we prove that the inclusion of two disjunctive multiplicity expressions is equivalent to the inclusion of the characterizing triples. Thus, we can view the characterizing triple as a normal form of a disjunctive multiplicity expression. Recall that $a \in w$ means that $w(a) \neq 0$.

Given a disjunctive multiplicity expression $E$, we define the characterizing triple ( $C_{E}, N_{E}, P_{E}$ ) consisting of the following sets:

- The conflicting pairs of siblings $C_{E}$ consists of pairs of symbols in $\Sigma$ such that $E$ defines no word using both symbols simultaneously:

$$
C_{E}=\left\{\left(a_{1}, a_{2}\right) \in \Sigma \times \Sigma \mid \nexists w \in L(E) . a_{1} \in w \wedge a_{2} \in w\right\} .
$$

- The extended cardinality map $N_{E}$ captures for each symbol in the alphabet the possible numbers of its occurrences in the unordered words defined by $E$ :

$$
N_{E}=\left\{(a, w(a)) \in \Sigma \times \mathbb{N}_{0} \mid w \in L(E)\right\} .
$$

- The sets of required symbols $P_{E}$ which captures symbols that must be present in every word; essentially, a set of symbols $X$ belongs to $P_{E}$ if every word defined by $E$ contains at least one element from $X$ :

$$
P_{E}=\{X \subseteq \Sigma \mid \forall w \in L(E) . \exists a \in X . a \in w\}
$$

As an example we take $E_{0}=a^{+}\|(b \mid c)\| d^{?}$. Because $P_{E}$ is closed under supersets, we list only its minimal elements:

$$
\begin{gathered}
C_{E_{0}}=\{(b, c),(c, b)\}, \quad P_{E_{0}}=\{\{a\},\{b, c\}, \ldots\}, \\
N_{E_{0}}=\{(b, 0),(b, 1),(c, 0),(c, 1),(d, 0),(d, 1),(a, 1),(a, 2), \ldots\} .
\end{gathered}
$$

An unordered word $w$ is consistent with the triple $\left(C_{E}, N_{E}, P_{E}\right)$ corresponding to a disjunctive multiplicity expression $E$, denoted $w \models\left(C_{E}, N_{E}, P_{E}\right)$ if $w$ is consistent with $C_{E}, N_{E}$, and $P_{E}$, respectively. Formally:

$$
\begin{aligned}
& w \models C_{E}:=\forall\left(a_{1}, a_{2}\right) \in C_{E} .\left(a_{1} \in w \Rightarrow a_{2} \notin w\right) \wedge\left(a_{2} \in w \Rightarrow a_{1} \notin w\right), \\
& w \models N_{E}:=\forall a \in \Sigma .(a, w(a)) \in N_{E}, \\
& w \models P_{E}:=\forall X \in P_{E} . \exists a \in X . a \in w .
\end{aligned}
$$

Furthermore, each element of a characterizing triple has a compact representation, which is polynomial in the size of the alphabet and computable in PTIME. Next, we present the construction for each compact representation:

- Given a disjunctive multiplicity expression $E=D_{1}^{M_{1}}\|\ldots\| D_{m}^{M_{m}}$, the size of $C_{E}$ is quadratic in $|\Sigma|$, but we can represent it linearly in $|\Sigma|$. Thus, we obtain $C_{E}^{*}$, which consists intuitively of non-singleton sets of labels from the same disjunction from $E$ such that the multiplicity associated to the disjunction is 1 :

$$
C_{E}^{*}=\left\{X \subseteq \Sigma_{D_{1}} \cup \ldots \cup \Sigma_{D_{m}} \mid \forall a, a^{\prime} \in X . a \neq a^{\prime} \Rightarrow\left(a, a^{\prime}\right) \in C_{E}\right\} .
$$

Then, $(a, b) \in \Sigma \times \Sigma$ belongs to $C_{E}$ iff one of the following holds: (i) there exists $X \in C_{E}^{*}$ s.t. $\{a, b\} \subseteq X$, or (ii) $a \notin \Sigma_{D_{1}} \cup \ldots \cup \Sigma_{D_{m}}$ or $b \notin \Sigma_{D_{1}} \cup \ldots \cup \Sigma_{D_{m}}$.

- Given a disjunctive multiplicity expression $E=D_{1}^{M_{1}}\|\ldots\| D_{m}^{M_{m}}$, note that the set $N_{E}$ may be infinite, but it can be represented in a compact manner using multiplicities: for any label $a$, the set $\left\{x \in \mathbb{N}_{0} \mid(a, x) \in N_{E}\right\}$ is representable by a multiplicity. Given a symbol $a \in \Sigma$, by $N_{E}^{*}(a)$ we denote the multiplicity $M$ such that $\llbracket M \rrbracket=\left\{x \in \mathbb{N}_{0} \mid(a, x) \in N_{E}\right\}$.

Moreover, for any $a \in \Sigma$, the multiplicity $N_{E}^{*}(a)$ can be easily obtained from $E$. More precisely:

$$
N_{E}^{*}(a)=\left\{\begin{array}{l}
0, \text { if } \forall i .1 \leqslant i \leqslant m \cdot a \notin \Sigma_{D_{i}}, \\
M^{a}, \text { if } \exists i .1 \leqslant i \leqslant m \cdot \Sigma_{D_{i}}=\{a\}, \\
?, \text { if } \exists i .1 \leqslant i \leqslant m . a \in \Sigma_{D_{i}} \wedge M_{i}=1 \wedge M^{a} \in\{?, 1\}, \\
*, \text { otherwise. }
\end{array}\right.
$$

Then, obviously, $(a, x) \in N_{E}$ iff $x \in \llbracket N_{E}^{*}(a) \rrbracket$.

- $P_{E}$ may be exponential in $|\Sigma|$, but it can be represented with its $\subseteq$-minimal elements:

$$
P_{E}^{*}=\left\{X \in P_{E} \mid \nexists X^{\prime} \in P_{E} . X^{\prime} \subset X\right\} .
$$

For a disjunctive multiplicity expression $E=D_{1}^{M_{1}}\|\ldots\| D_{m}^{M_{m}}$, $P_{E}^{*}$ consists intuitively of the disjunctions from $E$ such that the labels from the disjunction have multiplicities not accepting 0 occurrences. Therefore, we can construct $P_{E}^{*}$ in a straightforward manner:

$$
P_{E}^{*}=\left\{\Sigma_{D_{i}} \mid 1 \leqslant i \leqslant m \wedge \forall a \in \Sigma_{D_{i}} .0 \notin \llbracket M^{a} \rrbracket\right\} .
$$

Then $X \in P_{E}$ iff there exists $X^{\prime} \in P_{E}^{*}$ s.t. $X^{\prime} \subseteq X$.
For example, for the same $E_{0}=a^{+}\|(b \mid c)\| d^{?}$, we have:

$$
\begin{gathered}
C_{E_{0}}^{*}=\{\{b, c\}\}, \quad P_{E_{0}}^{*}=\{\{a\},\{b, c\}\}, \\
N_{E_{0}}^{*}(a)=+, \quad N_{E_{0}}^{*}(b)=N_{E_{0}}^{*}(c)=N_{E_{0}}^{*}(d)=?
\end{gathered}
$$

We also illustrate the construction of the compact representation of the characterizing triple on a more complex disjunctive multiplicity expression:

$$
E_{1}=(a \mid b)^{+}\left\|\left(c^{?}\left|d^{*}\right| e^{*}\right)\right\| f^{+}\left\|g^{?}\right\|\left(h^{+} \mid i\right)
$$

over the alphabet $\Sigma=\{a, b, c, d, e, f, g, h, i, j\}$. We obtain:

$$
\begin{gathered}
C_{E_{1}}^{*}=\{\{c, d, e\},\{h, i\}\}, \\
P_{E_{1}}^{*}=\{\{a, b\},\{f\},\{h, i\}\}, \\
N_{E_{1}}^{*}(a)=N_{E_{1}}^{*}(b)=N_{E_{1}}^{*}(d)=N_{E_{1}}^{*}(e)=N_{E_{1}}^{*}(h)=*, \\
N_{E_{1}}^{*}(c)=N_{E_{1}}^{*}(g)=N_{E_{1}}^{*}(i)=?, N_{E_{1}}^{*}(f)=+, N_{E_{1}}^{*}(j)=0 .
\end{gathered}
$$

We use the characterizing triple to give an alternative characterization of the membership of an unordered word to the language of a disjunctive multiplicity expression:
Lemma 4.1 An unordered word $w$ belongs to the language of a disjunctive multiplicity expression $E$ iff it is consistent with the triple $\left(C_{E}, N_{E}, P_{E}\right)$.
Proof For the if part, consider the triple $\left(C_{E}, N_{E}, P_{E}\right)$ corresponding to a normalized disjunctive multiplicity expression $E=D_{1}^{M_{1}}\|\ldots\| D_{m}^{M_{m}}$, and an unordered word $w$ such that $w \models\left(C_{E}, N_{E}, P_{E}\right)$. Let $w=w_{1} \uplus \ldots \uplus w_{m} \uplus w^{\prime}$, where, intuitively, each $w_{i}$ contains all the occurrences in $w$ of the symbols from $\Sigma_{D_{i}}$. Formally:

$$
\forall i .1 \leqslant i \leqslant m .\left(\left(\forall a \in \Sigma_{D_{i}} \cdot w_{i}(a)=w(a)\right) \wedge\left(\forall a^{\prime} \in \Sigma \backslash \Sigma_{D_{i}} \cdot w_{i}\left(a^{\prime}\right)=0\right)\right) .
$$

Since $w \models N_{E}$, we infer that $\forall a \in \Sigma \backslash\left(\Sigma_{D_{1}} \cup \ldots \cup \Sigma_{D_{m}}\right) . w(a)=0$, which implies that $w^{\prime}=\varepsilon$. Thus, proving $w \models E$ reduces to proving that $\forall i .1 \leqslant i \leqslant m$. $w_{i} \models D_{i}^{M_{i}}$. We prove while reasoning on each of the three possible forms of the disjunctions $D_{i}^{M_{i}}$, for every $i$ such that $1 \leqslant i \leqslant m$ :

1. $D_{i}^{M_{i}}=\left(a_{1}|\ldots| a_{n}\right)^{+}$, which implies that $\left\{a_{1}, \ldots, a_{n}\right\} \in P_{E}$. Since $w$ is consistent with $P_{E}$, we infer that $\exists j .1 \leqslant j \leqslant n . a_{j} \in w$. From the construction of $w_{i}$ we obtain $a_{j} \in w_{i}$, hence $w_{i} \models D_{i}^{M_{i}}$.
2. $D_{i}^{M_{i}}=\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right) \wedge \forall j .1 \leqslant j \leqslant n .0 \notin \llbracket M_{j} \rrbracket$. The form of $D_{i}^{M_{i}}$ and the definition of $N_{E}$ imply that:

$$
\forall j .1 \leqslant j \leqslant n . \forall x \in\{0\} \cup \llbracket M_{j} \rrbracket .\left(a_{j}, x\right) \in N_{E} .
$$

The form of $D_{i}^{M_{i}}$ and the definition of $P_{E}$ imply that $\left\{a_{1}, \ldots, a_{n}\right\} \in P_{E}$. Since $w$ is consistent with $P_{E}$ and $N_{E}$, we infer that $\exists j .1 \leqslant j \leqslant n$. $a_{j} \in w$, and, moreover, $w\left(a_{j}\right) \in$ $\llbracket M_{j} \rrbracket$.
The form of $D_{i}^{M_{i}}$ and the definition of $C_{E}$ imply that $\forall j, l \in\{1, \ldots, n\} .\left(j \neq l \Rightarrow\left(a_{j}, a_{l}\right) \in\right.$ $\left.C_{E}\right)$, which implies that $\forall j, l \in\{1, \ldots, n\} .\left(\left(j \neq l \wedge a_{j} \in w\right) \Rightarrow a_{l} \notin w\right)$.
From the last two relations we obtain that:

$$
\exists j .1 \leqslant j \leqslant n .\left(w_{i}\left(a_{j}\right) \in \llbracket M_{j} \rrbracket \wedge \forall l .1 \leqslant l \leqslant n .\left(l \neq j \Rightarrow a_{l} \notin w_{i}\right)\right)
$$

in other words we have shown that $w_{i} \models D_{i}^{M_{i}}$.
3. $D_{i}^{M_{i}}=\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right) \wedge \forall j .1 \leqslant j \leqslant n .0 \in \llbracket M_{j} \rrbracket$. The reasoning is similar to the previous case, the only difference is that now $\left\{a_{1}, \ldots, a_{n}\right\} \notin P_{E}$, so we obtain $w_{i} \models D_{i}^{M_{i}}$ even if none of the $a_{j}$ is present in $w_{i}$.
From the three cases presented above we conclude that $w \models\left(C_{E}, N_{E}, P_{E}\right) \Rightarrow w \models E$.
For the only if part, consider a normalized disjunctive multiplicity expression $E=D_{1}^{M_{1}} \|$ $\ldots \| D_{m}^{M_{m}}$ and an unordered word $w$ such that $w \models E$. This is equivalent to:

$$
\exists w_{1}, \ldots, w_{m} . w=w_{1} \uplus \cdots \uplus w_{m} \wedge \forall i .1 \leqslant i \leqslant m . w_{i} \models D_{i}^{M_{i}} .
$$

We prove that $E \models\left(C_{E}, N_{E}, P_{E}\right)$ while reasoning on the three cases for $D_{i}^{M_{i}}$, for every $i$ such that $1 \leqslant i \leqslant m$ :

1. $D_{i}^{M_{i}}=\left(a_{1}|\ldots| a_{n}\right)^{+}$. In this case $w_{i} \models D_{i}^{M_{i}}$ implies that $\exists j .1 \leqslant j \leqslant n$. $a_{j} \in w_{i}$, so $\left\{a_{1}, \ldots, a_{n}\right\} \in P_{E}$ is satisfied. There are no conflicting pairs of symbols in $\left\{a_{1}, \ldots, a_{n}\right\}$. Since $\forall j .1 \leqslant j \leqslant n . \forall x \in \mathbb{N}_{0} .\left(a_{j}, x\right) \in N_{E}$, we obtain that in $w_{i}$ all the symbols have numbers of occurrences consistent with $N_{E}$.
2. $D_{i}^{M_{i}}=\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right) \wedge \forall j .1 \leqslant j \leqslant n .0 \notin \llbracket M_{j} \rrbracket$. In this case $w_{i} \models D_{i}^{M_{i}}$ implies that:

$$
\exists j .1 \leqslant j \leqslant n .\left(w_{i}\left(a_{j}\right) \in \llbracket M_{j} \rrbracket \wedge \forall l .1 \leqslant l \leqslant n .\left(l \neq j \Rightarrow a_{l} \notin w_{i}\right)\right)
$$

which implies that $\left\{a_{1}, \ldots, a_{n}\right\} \in P_{E}$ is satisfied.
The conflicting pairs of symbols are also satisfied, more precisely we know from the form of $D_{i}^{M_{i}}$ and the definition of $C_{E}$ that $\forall j, l \in\{1, \ldots, n\} .\left(j \neq l \Rightarrow\left(a_{j}, a_{l}\right) \in C_{E}\right)$. Moreover, $w_{i} \models D_{i}^{M_{i}}$ implies that $\forall j, l \in\{1, \ldots, n\} .\left(j \neq l \wedge a_{j} \in w_{i} \Rightarrow a_{l} \notin w_{i}\right)$, so there are no conflicts in $w_{i}$.
From the form of $D_{i}^{M_{i}}$ and the definition of $N_{E}$, we know that:

$$
\forall j .1 \leqslant j \leqslant n . \forall x \in\{0\} \cup \llbracket M_{j} \rrbracket .\left(a_{j}, x\right) \in N_{E} .
$$

We infer that $w_{i}$ is consistent with $N_{E}$ for the present symbol (since $w_{i} \models D_{i}^{M_{i}}$ ) and also for the symbols which are not present (since 0 belongs to their extended cardinality map).
3. $D_{i}^{M_{i}}=\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right) \wedge \forall j .1 \leqslant j \leqslant n .0 \in \llbracket M_{j} \rrbracket$. In this case the reasoning for $C_{E}$ and $N_{E}$ is similar to the previous case. The difference is that now $P_{E}$ is less restrictive, since $\left\{a_{1}, \ldots, a_{n}\right\} \notin P_{E}$.

From the three cases presented above we conclude that $w \models E \Rightarrow w \models\left(C_{E}, N_{E}, P_{E}\right)$
We also characterize the inclusion of two languages given by the characterizing triples:
Lemma 4.2 Given two disjunctive multiplicity expressions $E_{1}$ and $E_{2}:\left(C_{E_{1}} \subseteq C_{E_{2}} \wedge N_{E_{2}} \subseteq\right.$ $\left.N_{E_{1}} \wedge P_{E_{1}} \subseteq P_{E_{2}}\right)$ iff $\left(\forall w . w \models\left(C_{E_{2}}, N_{E_{2}}, P_{E_{2}}\right) \Rightarrow w \models\left(C_{E_{1}}, N_{E_{1}}, P_{E_{1}}\right)\right)$.

Proof For the if part, we prove by contraposition:

- $C_{E_{1}} \nsubseteq C_{E_{2}} \Rightarrow \exists\left(a_{1}, a_{2}\right) \in C_{E_{1}} .\left(a_{1}, a_{2}\right) \notin C_{E_{2}} \Rightarrow \exists\left(a_{1}, a_{2}\right) \in \Sigma \times \Sigma$. ( $\exists w \in L\left(E_{1}\right) . a_{1} \in$ $\left.w \wedge a_{2} \in w\right) \wedge\left(\exists w^{\prime} \in L\left(E_{2}\right) . a_{1} \in w^{\prime} \wedge a_{2} \in w^{\prime}\right) \Rightarrow\left(\exists w^{\prime} . w^{\prime} \models C_{E_{2}} \wedge w^{\prime} \not \models C_{E_{1}}\right)$.
- $N_{E_{2}} \nsubseteq N_{E_{1}} \Rightarrow \exists a \in \Sigma . \exists w \in L\left(E_{2}\right)$. $\nexists w^{\prime} \in L\left(E_{1}\right) . w^{\prime}(a)=w(a) \Rightarrow\left(\exists w . w \models N_{E_{2}} \wedge w \not \models\right.$ $N_{E_{1}}$ ).
- $P_{E_{1}} \nsubseteq P_{E_{2}} \Rightarrow \exists X \subseteq \Sigma .\left(\forall w \in L\left(E_{1}\right) . \exists a \in X . a \in w\right) \wedge\left(\exists w^{\prime} \in L\left(E_{2}\right) . \forall a \in X . a \notin\right.$ $\left.w^{\prime}\right) \Rightarrow\left(\exists w^{\prime} . w^{\prime} \models L\left(E_{2}\right) \wedge w^{\prime} \not \vDash L\left(E_{1}\right)\right)$. Using the previous Lemma, we infer that $\left(\exists w^{\prime} . w^{\prime} \models P_{E_{2}} \wedge w^{\prime} \not \models P_{E_{1}}\right)$.

For the only if part, we take an unordered word $w$ such that $w \models\left(C_{E_{2}}, N_{E_{2}}, P_{E_{2}}\right)$ and we want to prove that $w \models\left(C_{E_{1}}, N_{E_{1}}, P_{E_{1}}\right)$, assuming that $C_{E_{1}} \subseteq C_{E_{2}}, N_{E_{2}} \subseteq N_{E_{1}}$, and $P_{E_{1}} \subseteq P_{E_{2}}$.

By definition, $w \models N_{E_{2}}$ implies that $\forall a \in \Sigma,(a, w(a)) \in N_{E_{2}}$. By hypothesis, $N_{E_{2}} \subseteq N_{E_{1}}$, therefore $\forall a \in \Sigma .(a, w(a)) \in N_{E_{1}}$, which by definition gives $w \models N_{E_{1}}$.

By definition, $w \models C_{E_{2}}$ implies that for all $(a, b) \in C_{E_{2}}$, (i) $(a \in w \Rightarrow b \notin w) \wedge(b \in w \Rightarrow a \notin w)$. By hypothesis, $C_{E_{1}} \subseteq C_{E_{2}}$, therefore (i) holds also for all $(a, b) \in C_{E_{1}}$, which by definition gives $w \models C_{E_{1}}$.

By definition, $w \models P_{E_{2}}$ implies that for all $X \in P_{E_{2}}$, (ii) $\exists a \in X$ s.t. $a \in w$. By hypothesis, $P_{E_{1}} \subseteq P_{E_{2}}$, therefore (ii) also holds for all $X \in P_{E_{1}}$, which by definition gives $w \models P_{E_{1}}$.

A consequence of Lemmas 4.1 and 4.2 is that the characterizing triples allow us to capture the containment of disjunctive multiplicity expressions:

Lemma 4.3 Given two disjunctive multiplicity expressions $E_{1}$ and $E_{2}, L\left(E_{2}\right) \subseteq L\left(E_{1}\right)$ iff $C_{E_{1}} \subseteq$ $C_{E_{2}}, N_{E_{2}} \subseteq N_{E_{1}}$, and $P_{E_{1}} \subseteq P_{E_{2}}$.

The above lemma shows that two equivalent disjunctive multiplicity expressions yield the same triples and hence the triple $\left(C_{E}, N_{E}, P_{E}\right)$ can be viewed as a normal form for the languages definable by a DMS. Formally:

Corollary 4.4 Given two disjunctive multiplicity expressions $E_{1}, E_{2}$, it holds that $L\left(E_{1}\right)=$ $L\left(E_{2}\right)$ iff $C_{E_{1}}=C_{E_{2}}, N_{E_{1}}=N_{E_{2}}$, and $P_{E_{1}}=P_{E_{2}}$.

### 4.1.3 Complexity results

From Lemma 4.3 we know that the containment of two disjunctive multiplicity expressions is equivalent to the containment of their characterizing triples. Next, we show that we can decide it in PTIME by using the compact representation of the characterizing triples:

Lemma 4.5 Given two disjunctive multiplicity expressions $E_{1}$ and $E_{2}$, deciding whether $L\left(E_{2}\right) \subseteq$ $L\left(E_{1}\right)$ is in PTIME.

Proof From Lemma 4.3 we know that, given two disjunctive multiplicity expressions $E_{1}$ and $E_{2}, L\left(E_{2}\right) \subseteq L\left(E_{1}\right)$ iff $C_{E_{1}} \subseteq C_{E_{2}}, N_{E_{2}} \subseteq N_{E_{1}}$, and $P_{E_{1}} \subseteq P_{E_{2}}$. Note that testing $N_{E_{2}} \subseteq N_{E_{1}}$ is equivalent to testing whether $\forall a \in \Sigma$. $N_{E_{2}}^{*}(a) \subseteq N_{E_{1}}^{*}(a)$, which is in PTIME since it reduces to manipulating multiplicities. Moreover, note that testing $P_{E_{1}} \subseteq P_{E_{2}}$ is equivalent to testing whether $\forall X \in P_{E_{1}}^{*} . \exists Y \in P_{E_{2}}^{*} . Y \subseteq X$, which is in PTIME since it reduces to testing the inclusion of a polynomial number of polynomial sets. On the other hand, we can decide $C_{E_{2}} \subseteq C_{E_{1}}$ in PTIME without using the compact representation because each of these sets has a number of elements quadratic in $|\Sigma|$, and can be easily computed in $O\left(|\Sigma|^{2}\right)$.

Furthermore, testing the containment of two DMS reduces to testing, for each symbol in the alphabet, the containment of the associated disjunctive multiplicity expressions. This problem is in PTIME (from Lemma 4.5). Hence, we obtain:

Theorem 4.6 $\mathrm{CNT}_{D M S}$ is in PTIME.
Next, we present the complexity results for satisfiability and membership, and a streaming algorithm for solving the membership. The problem of validating a XML document with bounded memory was addressed in [22, 23] and their conclusion is that constant memory validations can be performed only for some DTDs. We propose a streaming algorithm which processes an XML document in a single pass, using memory which depends on the height of the tree and not on its size. For a tree $t, h e i g h t(t)$ is the height of $t$ defined in the usual way. We employ the standard RAM model and assume that subsequent natural numbers are used as labels in $\Sigma$, startig with 1.

Proposition 4.7 Checking satisfiability of a DMS $S$ can be done in time $O\left(|\Sigma|^{2}\right)$. There exists a streaming algorithm that checks membership of a tree $t$ in a DMS $S$ in time $O\left(|\Sigma| \times|t|+|\Sigma|^{2}\right)$ and using space $O\left(\right.$ height $\left.(t) \times|\Sigma|+|\Sigma|^{2}\right)$.
The algorithm first checks satisfiability of the schema, by performing a preprocessing in time $O\left(|\Sigma|^{2}\right)$, and then a simple process based on dynamic programming. If the schema is not satisfiable, the algorithm rejects the tree w/o reading anything on the stream. Then the algorithm checks whether the schema is universal. A schema $S$ is universal if the $L\left(R_{S}\left(\operatorname{root}_{S}\right)\right)$ is the set of all unordered words over $\Sigma$. This can be performed in time $O\left(|\Sigma|^{2}\right)$. If we assume that $\Sigma=\left\{a_{1}, \ldots, a_{n}\right\}$, a simple algorithm has to check whether each normalized disjunctive multiplicity expression from the rules of the schema has the form $a_{1}^{*}\|\ldots\| a_{n}^{*}$.

For checking in streaming the membership of a tree $t$ to the language of a DMS $S$, the input tree $t$ is given in XML format. The algorithm works for any arbitrary ordering of sibling nodes. If the schema is universal, then the algorithm only reads the opening tag of the root of the tree. The tree is accepted if the label of the root is root ${ }_{S}$, and rejected otherwise. Otherwise, given a DMS $S$, in a preprocessing stage the algorithm constructs compact representations of the characterizing triples of the expressions used by $S$. Remark that, as DMS forbids repetition of symbols, the size of the representation of any expression is linear in $|\Sigma|$. Therefore, encoding the schema requires $O\left(|\Sigma|^{2}\right)$ space. For each symbol $a \in \Sigma$, we encode its corresponding rule using three global dictionaries, that we define as functions:

- cardinality ${ }_{a}: \Sigma \rightarrow\{0,1, ?,+, *\}$ which represents the extended cardinality map of the disjunctive multiplicity expression $R_{S}(a)$.
- conflict $_{a}: \Sigma \rightarrow\{0,1, \ldots,|\Sigma|\}$ which encodes the conflicts from $R_{S}(a)$ and has the following properties:
- For any disjunction of the form $\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right)$ from $R_{S}(a)$. conflict ${ }_{a}\left(a_{1}\right)=\ldots=$ conflict $_{a}\left(a_{n}\right) \wedge \forall a^{\prime} \in \Sigma . a^{\prime} \notin\left\{a_{1}, \ldots, a_{n}\right\}$. conflict $_{a}\left(a^{\prime}\right) \neq \operatorname{conflict}_{a}\left(a_{1}\right)$,
$-\forall a^{\prime} \in \Sigma . \forall X \in C_{R_{S}(a)}^{*} . a^{\prime} \notin X$. conflict $_{a}\left(a^{\prime}\right)=0$.
Let $\mathcal{C}_{a}=\left\{x \in\{0,1, \ldots,|\Sigma|\} \mid \exists a^{\prime} \in \Sigma\right.$. conflict $\left._{a}\left(a^{\prime}\right)=x\right\}$.
- required $_{a}: \Sigma \rightarrow\{0,1, \ldots,|\Sigma|\}$ which encodes the sets of required symbols from $R_{S}(a)$ and has the following properties:
- For any disjunction of the form $\left(a_{1}|\ldots| a_{n}\right)^{+}$or $\left(a_{1}^{M_{1}}|\ldots| a_{n}^{M_{n}}\right) .0 \notin \llbracket M_{1} \rrbracket$ from $R_{S}(a)$. required $_{a}\left(a_{1}\right)=\ldots=\operatorname{required}_{a}\left(a_{n}\right) \wedge \forall a^{\prime} \in \Sigma . a^{\prime} \notin\left\{a_{1}, \ldots, a_{n}\right\}$. required $_{a}\left(a^{\prime}\right) \neq$ required $_{a}\left(a_{1}\right)$,
$-\forall a^{\prime} \in \Sigma . \forall X \in P_{R_{S}(a)}^{*} . a^{\prime} \notin X$. required $_{a}\left(a^{\prime}\right)=0$.
Let $\mathcal{P}_{a}=\left\{x \in\{0,1, \ldots,|\Sigma|\} \mid \exists a^{\prime} \in \Sigma\right.$. required $\left._{a}\left(a^{\prime}\right)=x\right\}$.
For example, assume the rule $r \rightarrow(a \mid b)^{+}\left\|\left(c^{?}\left|d^{*}\right| e^{*}\right)\right\| f^{+}\left\|g^{?}\right\|\left(i \mid j^{+}\right)$over the alphabet $\Sigma=\{a, b, c, d, e, f, g, h, i, j\}$. A possible encoding is the following:

$$
\begin{gathered}
\operatorname{cardinality}_{r}(a)=\operatorname{cardinality}_{r}(b)=\operatorname{cardinality}_{r}(d)=\operatorname{cardinality}_{r}(e)=\operatorname{cardinality}_{r}(j)=*, \\
\operatorname{cardinality}_{r}(c)=\operatorname{cardinality}_{r}(g)=\operatorname{cardinality}_{r}(i)=?, \\
\operatorname{cardinality}_{r}(f)=+, \quad \operatorname{cardinality}_{r}(h)=0, \\
\operatorname{conflict}_{r}(a)=\operatorname{conflict}_{r}(b)=\operatorname{conflict}_{r}(f)=\operatorname{conflict}_{r}(g)=\operatorname{conflict}_{r}(h)=0, \\
\operatorname{conflict}_{r}(c)=\operatorname{conflict}_{r}(d)=\operatorname{conflict}_{r}(e)=1, \\
\operatorname{conflict}_{r}(i)=\operatorname{conflict}_{r}(j)=2, \\
\operatorname{required}_{r}(c)=\operatorname{required}_{r}(d)=\operatorname{required}_{r}(e)=\operatorname{required}_{r}(g)=\operatorname{required}_{r}(h)=0, \\
\operatorname{required}_{r}(a)=\operatorname{required}_{r}(b)=1, \quad \operatorname{required}_{r}(f)=2, \\
\operatorname{required}_{r}(i)=\operatorname{required}_{r}(j)=3 .
\end{gathered}
$$

During the execution, the algorithm maintains a stack whose height is the depth of the currently visited node. The bound on space required for stack operations is $O($ height $(t) \times|\Sigma|)$. We describe the local variables for each node $n \in N_{t}$, more precisely three dictionaries (with size linear in $|\Sigma|$ ) that we define as functions:

- count : $\Sigma \rightarrow\{0,1,2\}$ (initial value $=0$ ),
- present_conflict : $\mathcal{C}_{\text {lab }}^{t}(n) \backslash\{0\} \rightarrow \Sigma \cup\{0\}$ (initial value $=0$ ),
- present_required $: \mathcal{P}_{\text {lab }_{t}(n)} \backslash\{0\} \rightarrow\{0,1\}$ (initial value $=0$ ).

Next, we present Algorithms 1 and 2, which are executed when we encounter an opening or a closing tag, respectively. The streaming algorithm rejects a tree as soon as the opening tag is read for nodes that violate either some conflicting pair (Algorithm 1, lines 8-9) or the allowed cardinality (Algorithm lines 4-7). The algorithm also rejects a tree if at the closing tag of a node, there are children symbols required by the corresponding rule of the node's label and not present in its children list (Algorithm 2 lines 1-2). Unless the schema is universal (i.e., accepts any tree), the acceptance of a tree can be decided only after the closing tag of the root.

A streaming algorithm is called earliest if it produces its result at the earliest point. More precisely, consider the algorithm processing an XML stream of tree $t$ for checking membership of $t$ to a schema $S$. At each position of the stream (i.e. each opening or closing tag), the algorithm has seen a part of the tree $t$, and another part of $t$ remains unknown at that position. Let $p$ be some position of the stream. If the tree $t$ would be accepted (resp. rejected) whatever the

```
Algorithm 1 Procedure to execute when we are in a node \(n \in N_{t}\) and we encounter an open tag
of a node \(n_{a}\) labeled by \(a\).
algorithm open_tag \(\left(n_{a}\right)\)
Input: Open tag of a node \(n_{a} \in N_{t}\) labeled by \(a\)
Output: Reject the tree or update the local variables
    push on the stack the local variables for \(n_{a}\)
    if \(\operatorname{count}(a) \neq 2\) then
        \(\operatorname{count}(a):=\operatorname{count}(a)+1\)
    if \(\operatorname{count}(a)=2\) and \(\operatorname{cardinality}_{\operatorname{lab}_{t}(n)}(a) \notin\{+, *\}\) then
        reject
    if \(\operatorname{count}(a)=1\) and \(\operatorname{cardinality}_{\text {lab }_{t}(n)}(a)=0\) then
        reject
    if conflict \(_{\text {lab }_{t}(n)}(a) \neq 0\) and present_conflict conflict \(\left._{\text {lab }_{t}(n)}(a)\right) \notin\{0, a\}\) then
        reject
    if conflict \(_{l a b_{t}(n)}(a) \neq 0\) then
        present_conflict(conflict \(\left.{ }_{\text {lab }_{t}(n)}(a)\right):=a\)
    if required lab \(_{t}(n)(a) \neq 0\) then
        present_required \(\left(\operatorname{required}_{\text {lab }_{t}(n)}(a)\right):=1\)
```

```
Algorithm 2 Procedure to execute when we encounter the close tag of a node \(n \in N_{t}\).
algorithm close_tag( \(n\) )
Input: Close tag of a node \(n \in N_{t}\)
Output: Accept or reject the tree, or continue
    if \(\exists p \in \mathcal{P}_{\text {lab }_{t}(n)} \backslash\{0\}\). present_required \((p)=0\) then
        reject
    pop the local variables for \(n\) from the stack
    if \(n=\operatorname{root}_{t}\) then
        accept
```

part of $t$ unknown at position $p$, then an earliest streaming algorithm has to accept (resp. reject) the tree at position $p$. For example, if the language of the schema is universal, then an earliest algorithm would accept or reject the tree as soon as the opening tag of the root is read. It can be shown that the algorithm presented here is earliest.
We continue with complexity results that follow from known facts. Query satisfiability for DTDs is known to be NP-complete [4] and we adapt the result for DMS:

Proposition 4.8 $\mathrm{SAT}_{D M S, T w i g}$ is NP-complete.
Proof [sketch] Proposition 4.2.1 from [4] implies that satisfiability of twig queries in the presence of DTDs is NP-hard. We adapt the proof and we obtain the following reduction from 3SAT to $\operatorname{SAT}_{D M S, T w i g}$ : we take a $3 C N F$ formula $\varphi=\bigwedge_{i=1}^{n} C_{i}$ over the variables $x_{1}, \ldots, x_{m}$, where each $C_{i}$ is a disjunction of 3 literals. Consider $\Sigma=\left\{r, t_{1}, f_{1}, \ldots, t_{m}, f_{m}, C_{1}, \ldots, C_{n}\right\}$ and the corresponding tuple $(S, q)$ :

- The schema $S$ having the root label $r$ and the rules:
$-r \rightarrow\left(t_{1} \mid f_{1}\right)\|\ldots\|\left(t_{m} \mid f_{m}\right)$
$-t_{j} \rightarrow C_{j_{1}}\|\ldots\| C_{j_{k}}, 1 \leqslant j \leqslant m . x_{j}$ appears in $C_{j_{i}}$
$-f_{i} \rightarrow C_{j_{1}}\|\ldots\| C_{j_{k}}, 1 \leqslant j \leqslant m . \neg x_{j}$ appears in $C_{j_{i}}$
- The query $q=r\left[/ / C_{1}\right] \ldots\left[/ / C_{n}\right]$

For example, for the $3 C N F$ formula over the variables $x_{1}, \ldots, x_{4}: \varphi_{0}=\left(x_{1} \vee \neg x_{2} \vee x_{3}\right) \wedge\left(\neg x_{1} \vee\right.$ $x_{3} \vee \neg x_{4}$ ) we have the schema $S$ containing the rules:

$$
\begin{aligned}
& r \rightarrow\left(t_{1} \mid f_{1}\right)\left\|\left(t_{2} \mid f_{2}\right)\right\|\left(t_{3} \mid f_{3}\right) \|\left(t_{4} \mid f_{4}\right) \\
& t_{1} \rightarrow C_{1} \quad t_{3} \rightarrow C_{1} \| C_{2} \\
& f_{1} \rightarrow C_{2} \quad f_{3} \rightarrow \epsilon \\
& t_{2} \rightarrow \epsilon \quad t_{4} \rightarrow \epsilon \\
& f_{2} \rightarrow C_{1} \quad f_{4} \rightarrow C_{2}
\end{aligned}
$$

and the query:

$$
q=/ r\left[/ / C_{1}\right]\left[/ / C_{2}\right]
$$

The formula $\varphi$ is satisfiable iff $(S, q) \in \operatorname{SAT}_{D M S, T w i g}$. The described reduction works in polynomial time in the size of the input formula $\varphi$. Moreover, Theorem 4.4 from [4] implies that satisfiability of twig queries in the presence of DTDs is in NP, which yields the NP upper bound for $\mathrm{SAT}_{D M S, T w i g}$.

The complexity results for query implication and query containment in the presence of DMS follow from the EXPTIME-completeness proof from [19] for twig query containment in the presence of DTDs.

Proposition $4.9 \mathrm{IMPL}_{D M S, T \text { wig }}$ and $\mathrm{CNT}_{D M S, T \text { wig }}$ are EXPTIME-complete.
Proof [sketch] Theorem 4.4 from [19] implies that twig query containment in the presence of DTDs is in EXPTIME. This implies that the problems $\mathrm{IMPL}_{D T D, T w i g}, \mathrm{IMPL}_{D M S, T w i g}$, and $\mathrm{CNT}_{D M S, T \text { wig }}$ are also in EXPTIME. The EXPTIME-hardness proof of twig containment in the presence of DTDs (Theorem 4.5 from [19]) has been done using a reduction from Two-player corridor tiling problem and a technique introduced in [17]. In the proof from [19], when testing inclusion $p \subseteq_{S} q, p$ is chosen such that it satisfies any tree in $S$, hence $\mathrm{IMPL}_{D T D, T \text { wig }}$ is also

EXPTIME-complete. Furthermore, Lemma 3 in [17] can be adapted to twig queries and DMS: for any $S \in D M S$ and twig queries $q_{0}, q_{1}, \ldots, q_{m}$ there exists $S^{\prime} \in D M S$ and twig queries $q$ and $q^{\prime}$ such that:

$$
q_{0} \subseteq_{S} q_{1} \cup \ldots \cup q_{m} \Longleftrightarrow q \subseteq_{S^{\prime}} q^{\prime}
$$

Because the DTD in [19] can be captured with DMS, from the last two statements we conclude that $\mathrm{IMPL}_{D M S, T \text { wig }}$ and $\mathrm{CNT}_{D M S, T \text { wig }}$ are also EXPTIME-complete.

### 4.2 Disjunction-free multiplicity schema

In this subsection we present the static analysis for MS. Although query satisfiability and query implication are intractable for DMS, these problems become tractable for MS because they can be reduced to testing embedding of queries in some dependency graphs that we define in the sequel. We first present some of the technical tools which help us to reason about the disjunctionfree multiplicity schemas. Next, we use these tools to prove our results. Recall that MS use expressions of the form $a_{1}^{M_{1}}\|\ldots\| a_{n}^{M_{n}}$.

### 4.2.1 Dependency graphs

Definition 4.10 Given an $M S S=\left(\right.$ root $\left._{S}, R_{S}\right)$, the dependency graph of $S$ is a directed rooted graph $G_{S}=\left(\Sigma\right.$, root $\left._{S}, E_{S}\right)$ with the node set $\Sigma$, where root ${ }_{S}$ is the distinguished root node, and $(a, b) \in E_{S}$ if $R_{S}(a)=\ldots\left\|b^{M}\right\| \ldots$ and $M \in\{*,+, ?, 1\}$. Furthermore, the edge $(a, b)$ is called nullable if $0 \in \llbracket M \rrbracket$ (i.e., $M$ is $*$ or ?), otherwise ( $a, b$ ) is called non-nullable (i.e., $M$ is + or 1 ). The universal dependency graph of an $M S S$ is the subgraph $G_{S}^{\mathrm{u}}$ containing only the non-nullable edges.

In Figure 4 we present the dependency graphs for the schema $S_{5}$ containing the rules $r \rightarrow$ $a^{+} \| b^{*}, a \rightarrow b^{?}, b \rightarrow \epsilon$.


Figure 4: Dependency graph $G_{S_{5}}$ and universal dependency graph $G_{S_{5}}^{\mathrm{u}}$ for schema $S_{5}$.
An MS $S$ is pruned if $G_{S}^{\mathrm{u}}$ is acyclic. We observe that any MS has an equivalent pruned version which can be constructed in PTIME by removing the rules for the labels from which a cycle can be reached in the universal dependency graph. Note that a schema is satisfiable iff no cycle can be reached from its root in the universal dependency graph. From now on, we assume w.l.o.g. that all the MS that we manipulate are pruned.

We generalize the notion of embedding as a mapping of the nodes of a query $q$ to the nodes of a rooted graph $G=(\Sigma$, root,$E)$, which can be either a dependency graph or a universal dependency graph. Formally, an embedding of $q$ in $G$ is a function $\lambda: N_{q} \rightarrow \Sigma$ such that:

1. $\lambda\left(\operatorname{root}_{q}\right)=$ root,
2. for every $\left(n, n^{\prime}\right) \in \operatorname{child}_{q},\left(\lambda(n), \lambda\left(n^{\prime}\right)\right) \in E$,
3. for every $\left(n, n^{\prime}\right) \in \operatorname{desc}_{q},\left(\lambda(n), \lambda\left(n^{\prime}\right)\right) \in E^{+}$(the transitive closure of $E$ ),
4. for every $n \in N_{q}, l a b_{q}(n)=\star$ or $l a b_{q}(n)=\lambda(n)$.

If there exists an embedding from $q$ to $G$, we write $G \leqslant q$.

### 4.2.2 Graph simulation

A simulation of a rooted graph (either dependency graph or universal dependency graph) $G=$ $(\Sigma, r o o t, E)$ in a tree $t$ is a relation $R \subseteq \Sigma \times N_{t}$ such that:

1. $\left(\right.$ root, root $\left._{t}\right) \in R$
2. for every $(a, n) \in R,\left(a, a^{\prime}\right) \in E$, there exists $n^{\prime} \in N_{t}$ such that $\left(n, n^{\prime}\right) \in$ child $_{t}$ and $\left(a^{\prime}, n^{\prime}\right) \in R$
3. for every $(a, n) \in R . \operatorname{lab_{t}}(n)=a$

Note that $R$ is a total relation for the nodes of the graph reachable from the root i.e., for every $a \in \Sigma$ reachable from root in $G$, there exists a node $n \in N_{t}$ such that $(a, n) \in R$. If there exists a simulation from $G$ to $t$, we write $t \leqslant G$. The language of a graph is $L(G)=\{t \in$ Tree $\mid t \leqslant G\}$.

A rooted graph $G_{1}=\left(\Sigma\right.$, root, $\left.E_{1}\right)$ is a subgraph of another rooted graph $G_{2}=\left(\Sigma\right.$, root, $\left.E_{2}\right)$ if $E_{1} \subseteq E_{2}$. For a rooted graph $G=(\Sigma$, root, $E)$, we define the partial order $\leqslant_{G}$ on the subgraphs of $G$ : given $G_{1}$ and $G_{2}$ two subgraphs of $G, G_{1} \leqslant_{G} G_{2}$ if $G_{1}$ is a subgraph of $G_{2}$. Note that the relation $\leqslant_{G}$ is reflexive, antisymmetric, and transitive, thus being an order relation. Moreover, it is well-founded and it has a minimal element, that we denote $G_{0}$ for a graph $G$. Let $G_{0}=(\Sigma$, root, $\varnothing)$ and indeed, for any $G^{\prime}$ subgraph of $G$ we have $G_{0} \leqslant_{G} G^{\prime}$. In the sequel, we assume w.l.o.g. that all the subgraphs that we use in our proofs have the property that every edge can be part of a path starting at the root.

Lemma 4.11 For any disjunction-free multiplicity schema $S$, its universal dependency graph can be simulated in any tree $t$ which belongs to the language of $S$ :

$$
\forall S \in M S . \forall t \in L(S) . t \leqslant G_{S}^{\mathrm{u}}
$$

Proof Consider an MS $S$ and its universal dependency graph $G_{S}^{\mathrm{u}}$. Let $t$ be a tree which belongs to $L(S)$. We want to construct a witness relation $R \subseteq \Sigma \times N_{t}$ for $t \leqslant G_{S}^{\mathrm{u}}$ and the proof goes by induction on the structure of $G_{S}^{\mathrm{u}}$, using the well-founded order $\leqslant G_{S}^{u}$ defined above. Let $P(G)$ denote the statement $t \leqslant G$. Let $G$ be a subgraph of $G_{S}^{\mathrm{u}}$. The induction hypothesis is that for all $G^{\prime} \leqslant G_{S}^{\mathrm{u}} G$ and $G^{\prime} \neq G$, there exists a relation $R^{\prime}$ witness of the simulation $t \leqslant G^{\prime}$ and we are going to construct $R$ that witnesses $t \leqslant G$.

For the base case, we take the minimal element for the relation $\leqslant G_{S}^{u}$ let it $G_{0}=(\Sigma$, root, $\varnothing)$, then $P\left(G_{0}\right)$ holds for the relation $\left.R_{0}=\left\{\left(\text { root }^{\text {, root }}\right)_{t}\right)\right\}$, so the subgraph containing no edge can be simulated in $t$.

For the induction case, let $G$ a subgraph of $G_{S}^{\mathrm{u}}$. By the induction hypothesis, we know that $P\left(G^{\prime}\right)$ holds, for every $G^{\prime} \leqslant G_{S}^{u} G$. Consider a subgraph $G^{\prime}$ of $G$ such that $G$ contains exactly one additional edge w.r.t. $G^{\prime}$, let the additional edge ( $a, a^{\prime}$ ) and $R^{\prime}$ the witness relation for $t \leqslant G^{\prime}$. Because $G^{\prime} \leqslant G_{S}^{\mathrm{u}} G$ and $\left(a, a^{\prime}\right)$ is the only additional edge, we know that $R^{\prime}$ already contains images for $a$ in $t$ i.e., there exists a node $n$ such that $(a, n) \in R^{\prime}$. We construct the relation $R$ as the union of $R^{\prime}$ with $\left\{\left(a^{\prime}, n^{\prime}\right) \mid l a b_{t}\left(n^{\prime}\right)=a^{\prime} \wedge\left(\exists n .\left(n, n^{\prime}\right) \in \operatorname{child}_{t} \wedge(a, n) \in R^{\prime}\right)\right\}$. The set of tuples that we add is not empty because the edge ( $a, a^{\prime}$ ) belongs to the universal dependency graph $G_{S}^{\mathrm{u}}$, so for any node labeled by $a$ in the tree $t$ there exists a child of it labeled with $a^{\prime}$. The construction ensures that $R$ satisfies all the conditions of the definition of a simulation, so $t \leqslant G$, so $P(G)$ is true.

We have proved that $P\left(G_{0}\right)$ is true and that $\left(\forall G^{\prime} . G^{\prime} \leqslant G_{S}^{\mathrm{u}} G \Rightarrow P\left(G^{\prime}\right)\right) \Rightarrow P(G)$, so $P(G)$ is true for any $G$ subgraph of $G_{S}^{\mathrm{u}}$, so also for $G_{S}^{\mathrm{u}}$, hence $G_{S}^{\mathrm{u}}$ can be simulated into any tree $t$ which belongs to the language of $S$.

### 4.2.3 Graph unfolding

A path in a rooted graph (either dependency graph or universal dependency graph) $G=(\Sigma$, root,$E)$ is a non-empty sequence of vertices starting at root such that for any two consecutive vertices in the sequence, there is a directed edge between them in $G$. By Paths $(G) \subseteq \Sigma^{+}$we denote the set of all the paths in $G$. The set of paths is finite only for graphs without cycles reachable from the root. For instance, the paths of the graph $G_{1}$ in Figure 5(b) are $\operatorname{Paths}\left(G_{1}\right)=\{r, r a, r b, r c, r b d, r c d, r b d e, r c d e\}$.

Similarly, a path in a tree $t$ is a non-empty sequence of nodes starting at root $t_{t}$ such that any two consecutive nodes in the sequence are in the relation child. By Paths $(t)$ we denote the set of all the paths in $t$. Then, we define LabPaths $(t)$ as the set of sequences of labels of nodes from all the paths in $t$. For instance, for the tree $t_{1}$ from Figure 5(a) we have Paths $\left(t_{1}\right)=\left\{n_{0}, n_{0} n_{1}, n_{0} n_{1} n_{2}, n_{0} n_{3}, n_{0} n_{3} n_{4}\right\}$ and $\operatorname{LabPaths}\left(t_{1}\right)=\{r, r a, r a b\}$. Note that Paths $(t) \subseteq N_{t}^{+}, \operatorname{LabPaths}(t) \subseteq \Sigma^{+}$and $|\operatorname{LabPaths}(t)| \leqslant|\operatorname{Paths}(t)|$. The unfolding of a rooted graph $G=(\Sigma$, root, $E)$, denoted $u_{G}$, is a tree $u_{G}=\left(N_{u_{G}}\right.$, root $_{u_{G}}, l a b_{u_{G}}$, child $\left._{u_{G}}\right)$, such that:

- $N_{u_{G}}=\operatorname{Paths}(G)$,
- $\operatorname{root}_{u_{G}} \in N_{u_{G}}$ is the root of $u_{G}$,
- $(p, p . a) \in$ child $_{u_{G}}$, for all paths $p, p . a \in \operatorname{Paths}(G)$ (note that "." stands for concatenation),
- $l a b_{u_{G}}\left(\operatorname{root}_{u_{G}}\right)=$ root, and $l a b_{u_{G}}(p . a)=a$, for all the paths $p . a \in \operatorname{Paths}(G)$.

The unfolding of a graph is finite only when the graph has no cycle reachable from the root, because otherwise $\operatorname{Paths}(G)$ is infinite, so $u_{G}$ is infinite. In the sequel we use the unfolding for graphs without any cycle reachable from the root and in this case the unfolding is the smallest tree $u_{G}$ (w.r.t. the number of nodes) having $\operatorname{LabPaths}\left(u_{G}\right)=\operatorname{Paths}(G)$. The idea of the unfolding is to transform the rooted graph $G$ into a tree having the child relation instead of directed edges. There are nodes duplicated in order to avoid nodes with more than one incoming edge. For instance, in Figure 5(b) we take the graph $G_{1}$ and construct its unfolding $u_{G_{1}}$. We remark that the size of the unfolding may be exponential in the size of the graph, for example for the graph $G_{2}$ from Figure 5(c).

(a) Tree $t_{1}$.

(b) Graph $G_{1}$ and its unfolding.

(c) Graph $G_{2}$ and its exponential unfolding.

Figure 5: A tree and two graphs with their corresponding unfoldings.

### 4.2.4 Extending the definition of embedding

If a query $q$ can be embedded in a tree $t$, we may write $t \leqslant q$ instead of $t \models q$. We also extend the definition of embedding from a query to a tree to the embedding from a tree to another tree
i.e., given two trees $t$ and $t^{\prime}$, we say that $t^{\prime}$ can be embedded in $t$ (denoted $t \leqslant t^{\prime}$ ) if the query $\left(N_{t^{\prime}}\right.$, root $_{t^{\prime}}$, lab $_{t^{\prime}}$, child $\left._{t^{\prime}}, \varnothing\right)$ can be embedded in $t$. Similarly, we can define the embedding from a tree to a rooted graph. Note that two embeddings can be composed, for example:

- $\forall t, t^{\prime} \in$ Tree. $\forall q \in$ Twig. $\left(t \leqslant t^{\prime} \wedge t^{\prime} \leqslant q \Rightarrow t \leqslant q\right)$.
- $\forall S \in M S . \forall t \in$ Tree. $\forall q \in$ Twig. $\left(G_{S}^{(\mathrm{u})} \leqslant t \wedge t \leqslant q \Rightarrow G_{S}^{(\mathrm{u})} \leqslant q\right)$.

Lemma 4.12 A rooted graph (dependency graph or universal dependency graph) $G=(\Sigma$, root, $E$ ) can be simulated in a tree $t$ iff its unfolding $u_{G}$ can be embedded in $t$.

Proof For the if part, we know that $t \leqslant u_{G}$ so there exists a function $\lambda: N_{u_{G}} \rightarrow N_{t}$ which witnesses the embedding of $u_{G}$ in $t$. We construct a relation $R \subseteq \Sigma \times N_{t}$ such that:

$$
R=\left\{\left(\text { root }, \text { root }_{t}\right)\right\} \cup\left\{(a, n) \mid \exists p \in N_{u_{G}} \cdot p \cdot a \in N_{u_{G}} \wedge \lambda(p . a)=n\right\}
$$

This construction ensures that for every $(a, n) \in R$ and for every $\left(a, a^{\prime}\right) \in E$, there exists $n^{\prime} \in N_{t}$ such that $\left(n, n^{\prime}\right) \in$ child $_{t}$ and $\left(a^{\prime}, n^{\prime}\right) \in R$ because the function $\lambda$ is a witness for $t \leqslant u_{G}$ so the child relation is simply translated from $u_{G}$ to $G$. The construction of $R$ also guarantees that for every $(a, n) \in R$ we have $l a b_{t}(n)=a$ because $\lambda$ is the witness for $t \leqslant u_{G}$ and $\lambda(p . a)=n$. Thus we obtain that $R$ satisfies all the conditions to be a simulation of $G$ in $t$.

For the only if case, we take a relation $R$ which witnesses the simulation of $G$ in $t$. We construct the function $\lambda: N_{u_{G}} \rightarrow N_{t}$, witness of $t \leqslant u_{G}$, by recursion on the paths of $G$, because $\operatorname{Paths}(G)=N_{u_{G}}$. First of all, $\lambda\left(\operatorname{root}_{u_{G}}\right)=\operatorname{root}_{t}$. We assume that we have a recursive procedure which takes as input a path $p$, a label $a$, and the values of the function $\lambda$ computed before the procedure call, and it outputs $\lambda(p . a)$. The invariant of the procedure is that while defining $\lambda$ for $p . a, \lambda$ satisfies the conditions from the definition of embedding for all the nodes $\operatorname{root}_{u_{G}}, \ldots, p$ on the path to $p$. Furthermore, the values of $\lambda$ were obtained using the information given by $R$, so $\lambda(p)=n^{\prime}$ iff $R\left(l a b_{t}\left(n^{\prime}\right), n^{\prime}\right)$. Let $\lambda(p)=n^{\prime}$ and we construct $\lambda(p . a)=n$, where $R(a, n)$ and $\operatorname{child}_{t}\left(n^{\prime}, n\right)$. There exists such a node $n$ because of the recursive construction of $\lambda$ using $R$ and the invariant $\lambda(p . a)=n$ iff $R(a, n)$ is true. The construction of $\lambda$ ensures that $\lambda$ is root-preserving, child-preserving and label-preserving, so it satisfies all the conditions to be an embedding from $u_{G}$ to $t$, so we have found a correct witness for $t \leqslant u_{G}$.

Lemma 4.13 A query $q$ can be embedded in a rooted graph (dependency graph or universal dependency graph) $G$ iff $q$ can be embedded in the unfolding tree of $G$.

Proof For the if part, we know that $u_{G} \leqslant q$, so there exists a function $\lambda: N_{q} \rightarrow N_{u_{G}}$ witness of this embedding. We construct a function $\lambda^{\prime}: N_{q} \rightarrow \Sigma$, such that $\lambda^{\prime}(n)=l a b_{u_{G}}(\lambda(n))$ for each node $n$ from $N_{q}$. Since $\lambda$ is the witness of the embedding $u_{G} \leqslant q$, the constructed $\lambda^{\prime}$ satisfies all the conditions of the definition of an embedding from $q$ to $G$.

For the only if part, we know that $G \leqslant q$, so there exists a function $\lambda: N_{q} \rightarrow \Sigma$ witness of this embedding. We want to construct a function $\lambda^{\prime}: N_{q} \rightarrow N_{u_{G}}$ to prove $u_{G} \leqslant q$. We construct $\lambda^{\prime}$ by recursion on the tree structure of $q$. First of all, $\lambda^{\prime}\left(\operatorname{root}_{q}\right)=\operatorname{root}_{u_{G}}$. Then, the recursion hypothesis says that $G \leqslant q^{\prime}$ for any connected subtree $q^{\prime}$ obtained from $q$ by deleting some edges, $u_{G} \leqslant q^{\prime}$, which is witnessed by the function $\lambda^{\prime}$. Thus, for any node $n$ of $q, \lambda^{\prime}(n)=p$, where $p \in N_{u_{G}}$ because $N_{u_{G}}=\operatorname{Paths}(G)$ so any node in the unfolding can be identified by a unique sequence of labels among the paths of $G$. For the inductive case consider that $q$ is obtained from $q^{\prime}$ by adding one more edge, let it $\left(n, n^{\prime}\right)$. If it is a child edge and $\lambda^{\prime}(n)=p$, we construct $\lambda^{\prime}\left(n^{\prime}\right)=p \cdot \lambda\left(n^{\prime}\right)$, which is a path in $G$ by the definition of the unfolding. Otherwise, if it is a descendant edge and $\lambda^{\prime}(n)=p$, we construct $\lambda^{\prime}\left(n^{\prime}\right)=p \cdot p^{\prime} \cdot \lambda\left(n^{\prime}\right)$, where $p^{\prime}$ is a randomly chosen
path in $G$ from $\lambda(n)$ to $\lambda\left(n^{\prime}\right)$. We know by definition of $\lambda$ that such path exists. The construction ensures that $u_{G} \leqslant q$, for any $q$ satisfying the conditions of the recursion, so we can construct a function $\lambda^{\prime}$ which is a correct witness for $u_{G} \leqslant q$.

### 4.2.5 Fuse and add operations

In Figure 6] we present the operations fuse and add. We say that $t \triangleleft_{0} t^{\prime}$ if $t^{\prime}$ is obtained from $t$ by applying one of the operations from Figure 6. The fuse operation takes two siblings with the same label and creates only one node having below it the subtrees corresponding to each of the siblings. The $a d d$ operation consists simply in adding a subtree at any place in the tree. By $\unlhd$ we denote the transitive and reflexive closure of $\triangleleft_{0}$.



$\xrightarrow{\text { add }}$


Figure 6: Operations fuse and add.
Note that the fuse and add operations preserve the embedding i.e., given a twig query $q$ and two trees $t$ and $t^{\prime}$, if $t \leqslant q$ and $t \unlhd t^{\prime}$, then $t^{\prime} \leqslant q$. Furthermore, if we can embed a query $q$ in a tree $t$ which can be embedded in the dependency graph of an MS $S$, we can perform a sequence of operations such that $t$ is transformed into another tree $t^{\prime}$ satisfying $S$ and $q$ at the same time. Formally:

Proposition 4.14 Given an MS $S$, a query $q$ and a tree $t$, if $G_{S} \leqslant t$ and $t \leqslant q$, then there exists a tree $t^{\prime} \in L(S) \cap L(q)$. The tree $t^{\prime}$ can be constructed after a sequence of fuse and add operations (consistently with the schema $S$ ) from the tree $t$ and we denote $t \unlhd_{S} t^{\prime}$.

### 4.2.6 Family of characteristic graphs

Given a query $q$ and a schema $S$, if $q$ can be embedded in $G_{S}$ then we can capture all the trees satisfying $S$ and $q$ at the same time with a potentially infinite family of graphs. First, we explain the construction of the characteristic graphs. A characteristic graph $G$ for a schema $S$ and a query $q$ is a tuple $\left(V_{G}, \operatorname{root}_{G}, l a b_{G}, E_{G}\right)$, where $V_{G}$ is a finite set of vertices, $\operatorname{root}_{G} \in V_{G}$ is the root of the graph, $l a b_{G}: V_{G} \rightarrow \Sigma$ is a labeling function (with $l a b_{G}\left(\operatorname{root}_{G}\right)=\operatorname{root}_{S}$ ), and $E_{G} \subseteq V_{G} \times V_{G}$ represents the set of edges. Note that for two $x, y \in \Sigma \cup\{\star\}$ we say that $x$ matches $y$ if $y \neq \star$ implies $x=y$. We construct $G$ with the three steps described below:

1. For any $\left(n_{1}, n_{2}\right) \in \operatorname{child}_{q}$, add $n_{1}^{\prime}, n_{2}^{\prime}$ to $V_{G}$ and $\left(n_{1}^{\prime}, n_{2}^{\prime}\right)$ to $E_{G}$, where $l a b_{G}\left(n_{1}^{\prime}\right)$ matches $l a b_{q}\left(n_{1}\right)$ and $l a b_{G}\left(n_{2}^{\prime}\right)$ matches $l a b_{q}\left(n_{2}\right)$.
2. For any $\left(n_{1}, n_{2}\right) \in \operatorname{desc}_{q}$, choose an acyclic path $n_{1}^{\prime}, \ldots, n_{k}^{\prime}$ from $G_{S}$, such that $n_{1}^{\prime}$ matches $l a b_{q}\left(n_{1}\right)$ and $n_{k}^{\prime}$ matches $l a b_{q}\left(n_{2}\right)$. We add to $G$ the corresponding vertices and edges for this path, as shown for the previous case.
3. For any $n \in V_{G}$, take the subgraph from $G_{S}^{\mathrm{u}}$ starting at $l a b_{G}(n)$ and fuse it in the node $n$ in the graph $G$.

In Figure 7(b) we present an example of graph obtained from the embedding from Figure 7(a). We denote by $\mathcal{G}(q, S)$ the set of all the graphs obtained from a query $q$ and a disjunction-free multiplicity schema $S$ using the three steps above, using all the embeddings from $q$ into $S$. We extend the previous definition of the unfolding to the characteristic graphs. Since a graph $G \in \mathcal{G}(q, S)$ is acyclic, it has a finite unfolding. From the definition it also follows that the size of $G$ is polynomially bounded by $|q| \times|S|$ and $G \leqslant q$.

If we allow cyclic paths in step 2 , then we obtain similarly the set $\mathcal{G}^{*}(q, S)$. Note that $|\mathcal{G}(q, S)|$ is finite and may be exponential, while $\left|\mathcal{G}^{*}(q, S)\right|$ may be infinite. All the trees $t \in L(S) \cap L(q)$ can be obtained by fuse and add operations (consistently with $S$ ) from the unfolding trees of the graphs in $\mathcal{G}^{*}(q, S)$ :

$$
\forall t \in L(S) \cap L(q) . \exists G \in \mathcal{G}^{*}(q, S) . u_{G} \unlhd_{S} t
$$

Furthermore, by using a pumping argument, we have:

$$
\forall q \in \text { Twig. } \forall G \in \mathcal{G}^{*}(q, S) .\left(G 末 q \Rightarrow \exists G^{\prime} \in \mathcal{G}(q, S) . G^{\prime} \neq q\right) .
$$



Figure 7: An embedding from a query $q$ to a dependency graph $G_{S}$ and a graph $G \in \mathcal{G}(q, S)$. In $G_{S}$, the non-nullable edges are drawn with a full line and the nullable edges with a dotted line.

### 4.2.7 Complexity results

The dependency graphs and embeddings capture satisfiability and implication of queries by MS.

Lemma 4.15 For a twig query $q$ and an $M S S$ we have: 1) $q$ is satisfiable by $S$ iff $G_{S} \leqslant q$, 2) $q$ is implied by $S$ iff $G_{S}^{\mathrm{u}} \leqslant q$.

Proof [sketch] (1) For the if part, we know that $G_{S} \leqslant q$, so the family of graphs $\mathcal{G}(q, S)$ is not empty. The unfolding of any graph from $\mathcal{G}(q, S)$ satisfies $S$ and $q$ at the same time, hence $q$ is satisfiable by $S$.

For the only if part, we know that there exists a tree $t \in L(S) \cap L(q)$, which can for example be obtained after fuse operations (since one occurrence is consistent to all the multiplicities except 0 ) on the unfolding of a graph $G$ from $\mathcal{G}^{*}(q, S)$. Since $t \leqslant q$, we obtain $u_{G} \leqslant q$, so $G \leqslant q$, which, from the construction of $G$, implies that $G_{S} \leqslant q$.
(2) For the if part, we know that $G_{S}^{u} \leqslant q$, which implies by Lemma 4.13 that $u_{G_{S}^{u}} \leqslant q$. On the other hand, take a tree $t \in L(S)$. By Lemma 4.11 we have $t \leqslant G_{S}^{\mathrm{u}}$, which implies by Lemma 4.12 that $t \leqslant u_{G_{S}^{u}}$. From the last embedding and $u_{G_{S}^{u}} \leqslant q$ we infer that $t \leqslant q$. Since $t$ can be any tree in the language of $S$, we conclude that $q$ is implied by $S$.

For the only if part, we know that for any $t \in L(S), t \leqslant q$. Naturally, $u_{G_{S}^{u}}$ is in the language of $S$ (since one occurrence is consistent to all the multiplicities except 0 ), so $u_{G_{S}^{u}} \leqslant q$. From the definition of the unfolding, we can infer that $G_{S}^{\mathrm{u}} \leqslant u_{G_{S}^{\mathrm{u}}}$, which implies that $G_{S}^{\mathrm{u}} \leqslant q$.
Furthermore, testing the embedding of a query in a graph can be done in polynomial time with a simple bottom-up algorithm. From this observation and Lemma 4.15, we obtain:

Theorem $4.16 \mathrm{SAT}_{M S, T \text { wig }}$ and $\mathrm{IMPL}_{M S, \text { Twig }}$ are in PTIME.
The intractability of the containment of twig queries [17] implies the coNP-hardness of the containment of twig queries in the presence of MS. Proving the membership of the problem to coNP is, however, not trivial. Given an instance ( $p, q, S$ ), the set of all the trees satisfying $p$ and $S$ can be characterized with a set $\mathcal{G}(p, S)$ containing an exponential number of polynomially-sized graphs and $p$ is contained in $q$ in the presence of $S$ iff the query $q$ can be embedded into all the graphs in $\mathcal{G}(p, S)$. This condition is easily checked by a non-deterministic Turing machine.

## Theorem 4.17 $\mathrm{CNT}_{M S, T w i g}$ is coNP-complete.

Proof [sketch] Theorem 4 from [17] implies that $\mathrm{CNT}_{M S, T \text { wig }}$ is coNP-hard. Next, we prove the membership of the problem to coNP. Given an instance ( $p, q, S$ ), a witness is a function $\lambda: N_{p} \rightarrow \Sigma$. Testing whether $\lambda$ is an embedding from $p$ to $G_{S}$ requires polynomial time. If $\lambda$ is an embedding, a non-deterministic polynomial algorithm chooses a graph $G$ from $\mathcal{G}(p, S)$ and checks whether $q$ can be embedded in $G$. We claim that:

$$
p \not \Phi_{S} q \Longleftrightarrow \exists G \in \mathcal{G}(p, S) . G \nless q
$$

For the if case, we assume that there exists a graph $G \in \mathcal{G}(p, S)$ such that $G$. We know that $G \leqslant p$, so $u_{G} \leqslant p$, so there exists a tree $t \in L(S)$ such that $t \leqslant p$ and $u_{G} \unlhd_{S} t$ (using only fusions since one occurrence is consistent to all the multiplicities except 0 ). If we assume by absurd that $t \leqslant q$, we have $u_{G} \leqslant q$, so $G \leqslant q$, which is a contradiction. We infer thus that there exists a tree $t \in L(S) \cap L(p)$, such that $t \notin L(q)$, so $p \nsubseteq S q$.

For the only if case, we assume that $p \nsubseteq S q$, so there exists a tree $t \in L(S) \cap L(p)$ such that $t \notin L(q)$. Because $t \in L(S) \cap L(p)$, we know that there exists a graph $G \in \mathcal{G}^{*}(p, S)$, such that $u_{G} \unlhd_{S} t$. We know that $t \neq q$, so $u_{G} \not q$, so $G \nless q$. Moreover, we know using the pumping argument that in this case there exists a graph $G^{\prime} \in \mathcal{G}(p, S)$ such that $G^{\prime} \approx q$.

### 4.2.8 Extending the complexity results to disjunction-free DTDs

We also point out that the complexity results for implication and containment of twig queries in the presence of MS can be adapted to disjunction-free DTDs. This allows us to state results which, to the best of our knowledge, are novel.

Similarly to the MS, we represent a disjunction-free DTD as a tuple $S=\left(\operatorname{root}_{S}, R_{S}\right)$, where root $_{S}$ is a designed root label and $R_{S}$ maps symbols to regular expressions using no disjunction i.e., regular expressions of the form:

$$
E::=\varepsilon|a| E^{*}\left|E^{?}\right| E^{+} \mid E_{1} \cdot E_{2}
$$

where $a \in \Sigma$. Given such an expression $E$, consider the set non_nullable $(E)$ which contains the set of labels present in all the words from $L(E)$. Formally,

$$
\text { non_nullable }(E)=\left\{a \in \Sigma \mid \forall w \in L(E) . \exists w_{1}, w_{2} \cdot w=w_{1} \cdot a \cdot w_{2}\right\}
$$

We can compute non_nullable $(E)$ recursively:

```
non_nullable \((\varepsilon)=\) non_nullable \(\left(E^{*}\right)=\) non_nullable \(\left(E^{?}\right)=\varnothing\)
non_nullable \((a)=\{a\}\)
non_nullable \(\left(E_{1} \cdot E_{2}\right)=\) non_nullable \(\left(E_{1}\right) \cup\) non_nullable \(\left(E_{2}\right)\)
non_nullable \(\left(E^{+}\right)=\)non_nullable \((E)\)
```

Similarly, let nullable $(E)$ the set containing labels which appear in at least one word from $L(E)$. Formally,

$$
\operatorname{nullable}(E)=\left\{a \in \Sigma \mid \exists w \in L(E) . \exists w_{1}, w_{2} . w=w_{1} \cdot a \cdot w_{2}\right\}
$$

We can compute nullable $(E)$ recursively:

```
nullable \((\varepsilon)=\varnothing\)
nullable \((a)=\{a\}\)
\(\operatorname{nullable}\left(E^{+/ * / ?}\right)=\) nullable \((E)\)
\(\operatorname{nullable}\left(E_{1} \cdot E_{2}\right)=\operatorname{nullable}\left(E_{1}\right) \cup\) nullable \(\left(E_{2}\right)\)
```

Next, we adapt the notions of dependency graph and universal dependency graph for disjunctionfree DTDs. The dependency graph of a disjunction-free DTD $S$ is a rooted graph $G_{S}=$ $\left(\Sigma, \operatorname{root}_{S}, E_{S}\right)$, where

$$
E_{S}=\left\{\left(a, a^{\prime}\right) \mid a^{\prime} \in \operatorname{nullable}\left(R_{S}(a)\right)\right\} .
$$

Similarly, the universal dependency graph of a disjunction-free DTD $S$ is a rooted graph $G_{S}^{u}=$ $\left(\Sigma, \operatorname{root}_{S}, E_{S}^{\mathrm{u}}\right)$, where

$$
E_{S}^{\mathrm{u}}=\left\{\left(a, a^{\prime}\right) \mid a^{\prime} \in \text { non_nullable }\left(R_{S}(a)\right)\right\} .
$$

We assume w.l.o.g. that from now on we manipulate only disjunction-free DTDs having no cycle in the universal dependency graph. Otherwise, if there is a cycle in the universal dependency graph, this means that there does not exist any tree consistent with the schema and containing any of the labels implied in that cycle.

For a symbol $a \in \Sigma$ and a disjunction-free regular expression $E$, by $\min \_n b(E, a)$ we denote the minimum number of occurrences of the symbol $a$ in any word consistent with $E$.

```
\(\min \_n b(\varepsilon, a)=m i n \_n b\left(E^{*}, a\right)=\operatorname{min\_ nb}\left(E^{?}, a\right)=0\)
\(\min \_n b(a, a)=1\)
\(\operatorname{min\_ nb}\left(E_{1} \cdot E_{2}, a\right)=\operatorname{min\_ nb}\left(E_{1}, a\right)+\operatorname{min\_ nb}\left(E_{2}, a\right)\)
\(\operatorname{min\_ nb}\left(E^{+}, a\right)=m i n \_n b(E, a)\)
```

We adapt the definition of unfolding for the (universal) dependency graph of a disjunction-free DTD. For a disjunction-free multiplicity schema, the unfolding of the universal dependency graph belongs to its language since one occurrence is consistent with all the multiplicities except 0 . On the other hand, for a disjunction-free DTD $S$ this property does not hold, so we extend the construction of the unfolding with one more step:

- Let $u_{G_{S}^{\mathrm{u}}}$ be the unfolding of $G_{S}^{\mathrm{u}}$ obtained as it is defined for the MS.
- Update $u_{G_{S}^{u}}$ such that for any $n \in N_{u_{G_{S}^{\mathrm{u}}}}$, for any $a \in \Sigma$, let $t_{a}$ the subtree having as root the child of $n$ labeled by $a$. Next, add copies of $t_{a}$ as children of $n$ until $n$ has $\min \_n b\left(R_{S}\left(l a b_{u_{G_{S}^{u}}}(n)\right), a\right)$ children labeled with $a$.

Note that a consequence of this new definition is that the unfolding of the universal dependency graph of a disjunction-free DTD belongs to its language (modulo the order of the elements). The order imposed by the DTD on the elements is not important because in the sequel we work with twig queries, which ignore this order.

Proof [sketch] We claim that a query $q$ is implied by a disjunction-free DTD $S$ iff $G_{S}^{\mathrm{u}} \leqslant q$ and since the embedding of a query in a graph can be computed in polynomial time, this implies that IMPL ${ }_{\text {disj-free-DTD, Twig }}$ is in PTIME. The proof follows immediately from the proof of Lemma 4.15(2), taking into account the new definition of the unfolding. Theorem 4 from [17] implies that $\mathrm{CNT}_{\text {disj-free-DTD,Twig }}$ is coNP-hard. The membership of $\mathrm{CNT}_{\text {disj-free-DTD,Twig }}$ to coNP follows from the proof of Theorem 4.17, while taking into account the new definition of the unfolding.

## 5 Expressiveness of DMS

We compare the expressive power of DMS and DTDs with focus on schemas used in real-life applications. First, we introduce a simple tool for comparing regular expressions with disjunctive multiplicity expressions, and by extension, DTDs with DMS. For a regular expression $R$, the language $L(R)$ of unordered words is obtained by removing the relative order of symbols from every ordered word defined by $R$. A disjunctive multiplicity expression $E$ captures $R$ if $L(E)=$ $L(R)$. A DMS $S$ captures a DTD $D$ if for every symbol the disjunctive multiplicity expression on the rhs of a rule in $S$ captures the regular expression on the rhs of the corresponding rule in $D$. We believe that this simple comparison is adequate because if a DTD is to be used in a data-centric application, then supposedly the order between siblings is not important. Therefore, a DMS that captures a given DTD defines basically the same type of admissible documents, without imposing any order among siblings. Naturally, if we use the above notion to compare the expressive powers of DTDs and DMS, DTDs are strictly more expressive than DMS.

We use the comparison on the XMark [20] benchmark and the University of Amsterdam XML Web Collection [13]. We find that all 77 regular expressions of the XMark benchmark are captured by DMS rules, and among them 76 by MS rules. As for the DTDs found in the University of Amsterdam XML Web Collection, $84 \%$ of regular expressions (with repetitions discarded) are captured by DMS rules and among them $74.6 \%$ by MS rules. Moreover, $55.5 \%$ of full DTDs in the collection are captured by DMS and among them $45.8 \%$ by MS. Note that these figures should be interpreted with caution, as we do not know which of the considered DTDs were indeed intended for data-centric applications. We believe, however, that these numbers give a generally positive answer to the question of how much of the expressive power of DTDs the proposed schema formalisms, DMS and MS, retain.

## 6 Conclusions and future work

We have studied the computational properties and the expressive power of new schema formalisms, designed for unordered XML: the disjunctive multiplicity schema (DMS) and its restriction, the disjunction-free multiplicity schema (MS). DMS and MS can be seen as DTDs
using restricted classes of regular expressions and interpreted under commutative closure to define unordered content models. These restrictions allow on the one hand to maintain a relatively low computational complexity of basic static analysis problems while retaining a significant part of expressive power of DTDs.

An interesting question remains open: are these the most general restrictions that allow to maintain a low complexity profile? We believe that the answer to this question is negative and intend to identify new practical features that could be added to DMS and MS. One such feature are numeric occurrences [14] of the form $a^{[n, m]}$ that generalize multiplicities by requiring the presence of at least $n$ and no more than $m$ elements $a$. It would also be interesting to see to what extent our results can be used to propose hybrid schemas that allow to define ordered content for some elements and unordered model for others.

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